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Conventional Weapons Demilitarization: A Health and Environmental Effects Data Base Assessment

Methods for Estimating Multi-Pathway Exposures to Environmental Contaminants

Final Report, Phase II

T. E. McKone

June 1988

Lawrence Livermore National Laboratory

Supported by
U.S. Army Medical Research and Development Command
Fort Detrick, Frederick, MD 21701-5012
Project Order 83PP3818
Project Officer: Mitchell J. Small

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UNCLASSIFIED
SECURITY CLASSIFICATION OF THIS PAGE

REPORT DOCUMENTATION PAGE

Form Approved OMB No. 0704-0188

1a REPORT SECURITY CLASSIFICATION: UNCLASSIFIED	1b RESTRICTIVE MARKINGS
2a SECURITY CLASSIFICATION AUTHORITY	3 DISTRIBUTION/AVAILABILITY OF REPORT: Approved for public release; distribution unlimited
2b DECLASSIFICATION/DOWNGRADING SCHEDULE	
4 PERFORMING ORGANIZATION REPORT NUMBER(S): UCRL-21064	5 MONITORING ORGANIZATION REPORT NUMBER(S)
6a NAME OF PERFORMING ORGANIZATION: Lawrence Livermore National Laboratory; 6b OFFICE SYMBOL (If applicable)	7a NAME OF MONITORING ORGANIZATION: U.S. Army Medical Bioengineering Research and Development Laboratory
6c ADDRESS (City, State, and ZIP Code): Environmental Sciences Division, P.O. Box 5507, Livermore, CA 94550	7b ADDRESS (City, State, and ZIP Code): ATTN: SGRD-UB7-C, Fort Detrick, Fredrick, MD 21701-5010
8a NAME OF FUNDING/SPONSORING ORGANIZATION: U.S. Army Medical Research & Development Command; 8b OFFICE SYMBOL (If applicable): SGRD-RMI-S	9 PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER: Army Project Order 83PP3818
8c ADDRESS (City, State, and ZIP Code): Fort Detrick, Fredrick, MD 21701-5012	10 SOURCE OF FUNDING NUMBERS: PROGRAM ELEMENT NO. 62720A; PROJECT NO. 3E1-62720A835; TASK NO. AA; WORK UNIT ACCESSION NO. 006
11 TITLE (Include Security Classification): Conventional Weapons Demilitarization: A Health and Environmental Effects Data Base Assessment	
12 PERSONAL AUTHOR(S): McKone, T.E.	
13a TYPE OF REPORT: Final, Phase II; 13b TIME COVERED: FROM _____ TO _____; 14 DATE OF REPORT (Year, Month, Day): June 1988; 15 PAGE COUNT: 102	
16 SUPPLEMENTARY NOTATION: Subtitle: Methods for Estimating Multi-Pathway Exposures to Environmental Contaminants	

17 COSATI CODES			18 SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
FIELD	GROUP	SUB-GROUP	
5	06		Exposure modelling, multimedia pollution, pathway exposure factors, innalation exposure, ingestion exposure, dermal exposure.
5	09		

19 ABSTRACT (Continue on reverse if necessary and identify by block number)

This report describes a model that expresses human exposure using multiple exposure pathways linked to multiple environmental media. Starting with contaminant concentrations in air (as gases or attached to particles), water, and soil; the model links human exposure through innalation, ingestion, and dermal absorption to concentrations in each environmental compartment. The concentration in a specific compartment is linked to exposure through a specific pathway using a pathway exposure factor (PEF). The PEF is a numerical expression that incorporates information on human physiology and lifestyle together with models of environmental partitioning into an expression that translates a unit concentration (mg/m^3 in air, mg/L in water, or mg/kg in soil) into a daily exposure in mg/kg-d for a specific pathway. Human, animal, and environmental data used in calculating PEFs are presented and discussed. The report provides a detailed derivation of PEFs for air/inhalation, air/ingestion, soil/inhalation, soil/ingestion, soil/dermal absorption, water/inhalation, water/ingestion, and water/dermal absorption pathways. The model is illustrated by sample applications of hypothetical arsenic, benzene, and trinitrotoluene (TNT) contamination.

20 DISTRIBUTION/AVAILABILITY OF ABSTRACT: ☐ UNCLASSIFIED/UNLIMITED ☒ SAME AS RPT ☐ DTIC USERS	21 ABSTRACT SECURITY CLASSIFICATION: UNCLASSIFIED
22a NAME OF RESPONSIBLE INDIVIDUAL: Mary Francis Bostian	22b TELEPHONE (Include Area Code): (301) 663-7325; 22c OFFICE SYMBOL: SGRD-RMI-S

DD Form 1473, JUN 86 — Previous editions are obsolete.

SECURITY CLASSIFICATION OF THIS PAGE
UNCLASSIFIED

AD
UCRL-21064

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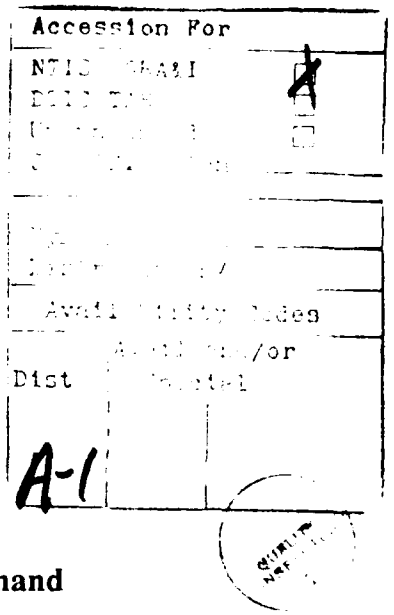

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CONTENTS

Preface

This report is one in a series of reports that addresses the environmental health risks associated with demilitarization of conventional ordnance. These reports have been prepared by Lawrence Livermore National Laboratory through the support of the U.S. Army Biomedical Research and Development Laboratory. These reports have been produced through a study that has been conducted in two phases. In Phase I, demilitarization technologies were examined along with their solid, liquid, and gaseous effluents. The by-products were then ranked according to their potential health and environmental effects. In Phase II, data-base assessments have been completed on the environmental chemistry, toxicology, and effects of explosives, propellants, and their associated co-contaminants. The Phase I study produced two reports — "Demilitarization of Conventional Ordnance: Priorities for Data-Base Assessments of Environmental Contaminants" (Layton et al., 1986) and "GEOTOX Multimedia Compartment Model User's Guide" (McKone et al., 1987). The current report builds on the models and data presented in the Phase I reports and complements the data that will be presented in the other Phase II reports.

1. INTRODUCTION

Historically, the primary methods for destroying explosives and propellants have been to burn or detonate them at secure sites. Open-burning and open-detonation (OB/OD) operations, as they are termed, can result in the contamination of soils and ground waters adjacent to OB/OD operations. The regulation of OB/OD comes under Subpart X of the Resource Conservation and Recovery Act (RCRA). In 1987 the U.S. Environmental Protection Agency (U.S. EPA) adopted a final rule covering the kinds of information and analyses needed to obtain a RCRA permit for these operations (U.S. EPA, 1987a). The U.S. EPA adopted a flexible approach for regulatory OB/OD because of the diverse nature of such operations and the recognition that no one approach could successfully protect human health and the environment. A fundamental goal of the analyses supporting a permit for an OB/OD regulation is to demonstrate that human health would not be adversely affected. This may be demonstrated in various ways, for example, by showing that all applicable standards will be met or that residual contaminants will be effectively contained. Risk-based assessments can also play an important role in determining whether an OB/OD operation poses unacceptable risks. A key component of a risk assessment is an estimation of potential human exposures to residual contaminants in different media. The results of an exposure assessment are subsequently used with toxicity data to analyze the nature and magnitude of potential health risks to individuals.

The goal of this report is to present a framework for analyzing exposures resulting from contaminant exposures via different pathways. Our approach is oriented toward the preparation of preliminary estimates of exposures to contaminants, but it can be easily adapted to site-specific assessments. The techniques presented are consistent with the U.S. EPA guidelines for preparing exposure assessments (see U.S. EPA, 1987b).

A realistic strategy for managing the health risks of environmental contaminants requires a comprehensive and integrated assessment of human exposures. According to the U.S. EPA (U.S. EPA, 1987b) exposure can be defined as "the contact with a chemical or physical agent. The magnitude of the exposure is determined by measuring or estimating the amount of an agent available at the exchange boundaries, i.e., lungs, gut, or skin during some specified time." This report presents a methodology and supporting data that address several potential exposure pathways and provides a link between

human exposure and chemical concentrations in multiple environmental media. This approach links environmental concentrations to human exposure through pathway exposure factors (PEFs). The PEF incorporates information on human physiology, human behavior patterns, and environmental transport into a term that translates a unit concentration (in mg/m^3, mg/kg, or mg/L) in a specified environmental medium (such as air, soil, or water) into daily exposure in mg/kg-d for a specified route (such as inhalation, ingestion, or dermal absorption). Each PEF links the contaminant concentration in a given medium with the exposure through a specific pathway. For example, the PEF that links water concentration to dermal absorption converts a water supply concentration in mg/L into dermal absorption exposure in mg/kg-d for the population using the water supply.

This report addresses human exposure through nine different routes:

1) inhalation,
2) ingestion of water,
3) ingestion of fruits and vegetables,
4) ingestion of grains,
5) ingestion of meat,
6) ingestion of milk,
7) ingestion of fish,
8) ingestion of soil, and
9) dermal absorption.

These exposure pathways are linked to environmental concentrations in five environmental media:

1) outdoor air (gases),
2) outdoor air (particles),
3) soil,
4) ground water, and
5) surface water.

Table 1-1 lists the matrix of PEFs that are used to link the nine exposure pathways with the five environmental media. The procedures outlined in this report are compatible with the GEOTOX model that we developed to simulate the transport and fate of demilitarization by-products (see Layton et al., 1986). The GEOTOX model explicitly calculates concentrations for the

Table 1-1. Matrix of environmental concentrations and pathway exposure factors.

Pathways	Environmental concentrations[a] Air (gas phase) C_a	Air (particles) C_p	Soil C_s	Potable water[b] C_w	Surface water C_r
Inhalation	F_{aa}	F_{pa}	F_{sa}	F_{wa}	--
Ingestion					
Water	--		--	F_{ww}	--
Fruits and Vegetables	F_{av}	F_{pv}	F_{sv}	--	--
Grains	F_{ag}	F_{pg}	F_{sg}	--	--
Meat	F_{at}	F_{pt}	F_{st}	F_{wt}	--
Milk	F_{ak}	F_{pk}	F_{sk}	F_{wk}	--
Fish	--	--	--	--	F_{rf}
Soil	--	--	F_{ss}	--	--
Dermal absorption	--	--	F_{sd}	F_{wd}	--

[a] Subscripts refer to the source media (a = air (gases), p = air (particles), s = soil, w = potable water and r = surface water) and pathways (a = inhalation, w = water, v = vegetables, g = grain, t = meat, k = milk, f = fish, s = soil ingestion, and d = dermal absorption).

[b] Potable-water concentrations are obtained from combining the concentrations in surface and ground water so as to reflect the mix in the local-water supply.

five environmental media just mentioned. Nevertheless, it is equally feasible to obtain the required input concentrations from direct measurement or simulations using medium-specific models (e.g., air dispersion, ground-water transport, etc.).

The remainder of this report is divided into six sections. The first of these, Section 2, provides background discussions on obtaining environmental concentrations; the relation between exposure, dose, and risk; data on human anatomical and dietary parameters; and data on cattle relevant to calculations of exposure to meat and dairy products.

Section 3 provides a discussion of exposure routes associated with contaminants, including both gases and particles, in ambient outdoor air. This section covers the relationship between indoor and outdoor air concentrations; deposition of particles and gases onto vegetation for transfer to food; and the transfer of airborne contaminants from air to meat and milk as a result of inhalation and ingestion by cattle of gases and particles deposited onto the surface of vegetation.

Section 4 deals with the transfer of contaminants from soil to humans through ingestion and indoor inhalation. Transfer of contaminants to indoor air is attributable to soil/dust transfers from humans and their pets. We consider the ingestion of soil by both children and adults. Contaminants are transferred to meat and milk through the ingestion by cattle of contaminated soil and plant tissues. We also consider the transfer of contaminants to food supplies from soil to food crops; including vegetables, grains, and fruits. Finally, dermal absorption from contaminated soil on skin surfaces is considered.

The next section, Section 5, addresses human exposures associated with the transfer of contaminants from ground and surface water to potable-water supplies. In this section, we develop PEFs for the transfer of contaminants from surface water to fish and from water supplies derived from ground or surface water to drinking water, to meat and milk from water ingestion by animals, to indoor air from household water use, and to skin through dermal absorption.

Section 6 provides a summary and discussion of the methods presented in this report. This section also provides a sample calculation that is used to illustrate the use of the PEFs.

Figure 1-1 illustrates the integration between environmental transport and transformation processes and the assessment of human exposure. The exposure pathways addressed in this report are identified by ovals at the top of the diagram. These pathways are connected to the environmental compartments that directly affect the levels of exposure. The compartments that affect exposure directly are identified as solid boxes. Contaminant concentrations in these compartments are needed as inputs to the exposure model and can be obtained through either modelling or measurement. Contaminant concentrations in the solid boxes are influenced by transport and transformation in the total environment. Boxes enclosed by dotted lines

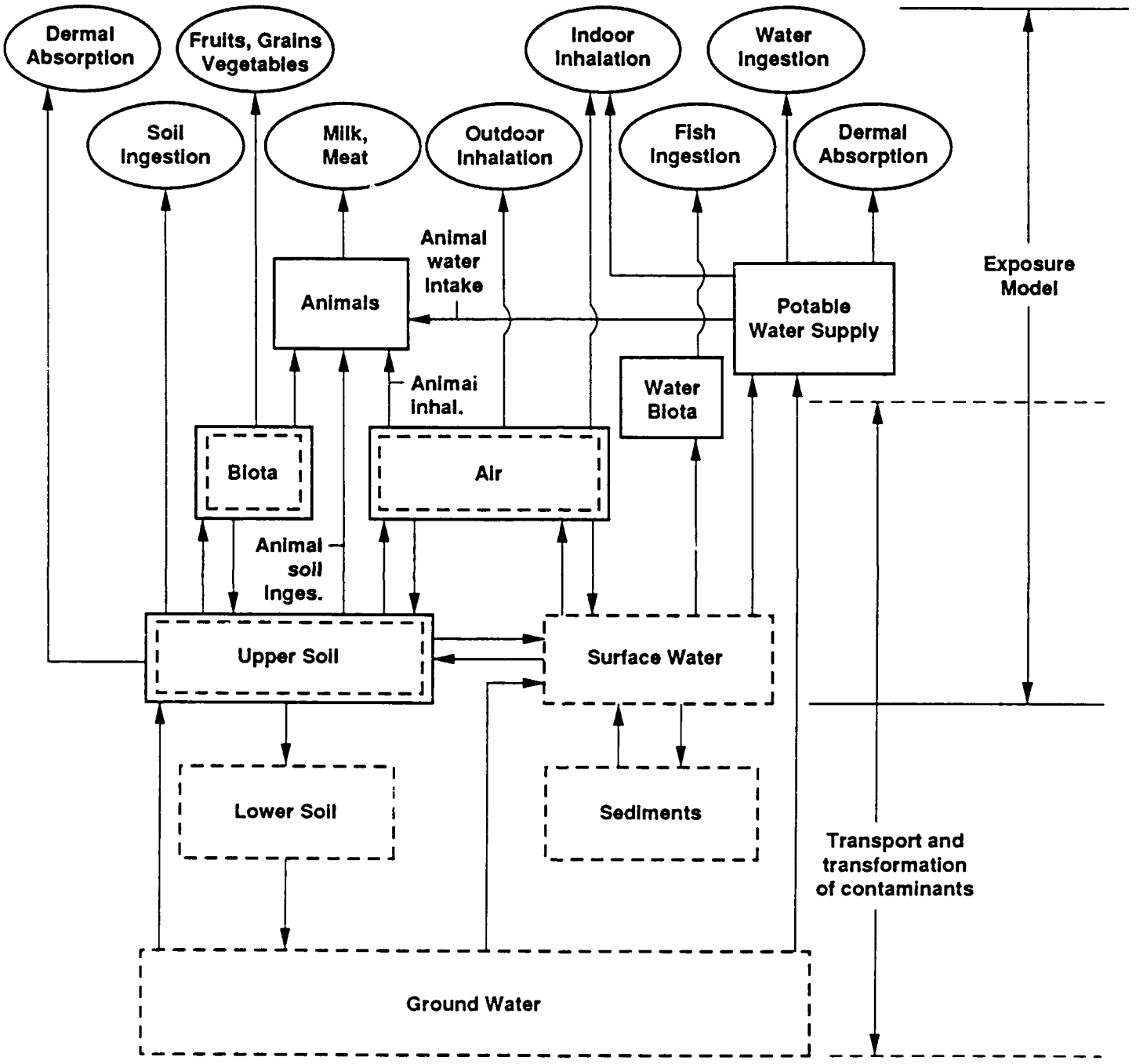

Figure 1-1. Integration between environmental transport and transformation processes and the assessment of human exposure.

represent the environmental compartments that must be considered when one evaluates the environmental fate of a contaminant species. The process for modelling chemical exchange among these compartments is described in Layton et al. (1986); McKone et al. (1987); and McKone and Layton (1986).

2. BACKGROUND: THE RELATIONSHIP OF ENVIRONMENTAL CONCENTRATIONS TO EXPOSURE AND HEALTH RISK

Assessment of human exposure to environmental contaminants is a process that translates environmental concentrations into quantitative estimates of the amount of chemical that passes through the lung linings, skin surface, and gut wall of individuals within a specified population. This quantity is used as a basis for projecting the incidence of health detriment within the population. The process of estimating exposure using often limited data and extrapolating to a large diverse population requires many assumptions, inferences, and simplifications. How well the resulting exposure estimates reflect actual exposures is largely an unanswerable question. There are many sources of uncertainty, and many of the uncertainties defy quantification. Nevertheless, the process of exploring the data and proposing an exposure model gives us the opportunity to evaluate and compare the processes by which environmental contaminants can lead to health effects within human populations. An important product of such an exercise is to provide guidance on where further research is needed to enhance the data or alter methods. In addition, these estimates provide risk managers and the affected population with insight that can help in evaluating proposed risk management actions.

This section provides background material for the remainder of the report and addresses general issues that should be resolved before proceeding to detailed technical calculations for exposure assessments. We begin with a discussion of environmental concentrations (e.g., units, measurements, and simulation). In the remaining sections of the report information on media-specific concentrations of a contaminant is assumed to be available and in the proper units. The terms exposure, dose, and risk are defined and a brief overview on how these concepts interact is provided. Following this is an overview on human anatomical and dietary parameters that will be used in later sections. Finally, we review data on cattle that are relevant for calculations of meat and dairy-product exposures.

ENVIRONMENTAL CONCENTRATIONS

The exposure models described in this report require contaminant concentrations in five environmental media:

(1) concentrations in the gas phase of outdoor air,

(2) concentrations in the particulate phase of outdoor air,

(3) soil concentrations,

(4) ground-water concentrations, and

(5) surface-water concentrations.

Before assessing exposure, one must obtain these concentrations either through measurement or modelling. In addition, it is important to establish a protocol for the units expressing these concentrations.

Units

Air. Contaminants in air can occur as a result of their attachment to soil or other particles suspended in air or as part of the atmospheric gas phase. For purposes of exposure estimates, air concentrations are expressed as mg(contaminant)/m^3(air) and divided into two fractions--a gas fraction, C_a, and a fraction attached to atmospheric particles, C_p.

Soil. Soil is composed of liquid, solid, and gas phases. According to Bowen (1979), roughly 80% of the soil mass is composed of solid particles and roughly 20% is composed of soil solution. By volume, soils are on the order of 60% solid, 10 to 30% water, and 10 to 30% air. For purposes of estimating exposure, we use the total contaminant concentration in the combined liquid and solid phases as the representative value, C_s in mg(contaminant)/kg(soil), for expressing soil concentration.

Water. The contaminant concentration in ground water, C_g, includes only the dissolved component and the suspended particles that will pass through 45 μm filters (this approximates the efficiency of natural filtering). The contaminant concentration in surface water, C_r, includes both the dissolved contaminant and the amount of contaminant attached to suspended sediment. In the potable-water supply, the contaminant concentration, C_w, includes both

dissolved contaminant and the suspended contaminant that are not removed prior to entering public water supplies. C_w, C_g, and C_r are in units of mg(contaminant)/L(water).

Biota. The concentration of a contaminant in biota is obtained from either direct assessment of biota concentrations or indirectly by relating the biota concentration to the soil concentration using the plant/soil partitioning factor, K_{sp} (see Layton et al., 1986). In either case the biota concentration is likely to be expressed in mg(contaminant)/kg(plant dry mass). However, much of the data on dietary uptake uses food consumption data expressed in kg(fresh mass)/d. In this report, we use biota concentrations expressed in mg/kg (dry mass) or mg/kg (DM) and convert when necessary. According to Bowen (1979) the ratio kg(DM)/kg(fresh mass) is 0.3 for the biosphere. Small (1984) reports this value as 0.15 for edible plants. We use 0.3 as the dry mass fraction for pasture grasses and 0.2 as the dry mass fraction for fruits, vegetables, and grains.

Measured Values

When proceeding from measured concentration values to exposure estimates, one should be able to characterize the time period and geographical region that are reflected in the measured values. For example, atmospheric concentrations should be measured over a long enough period to provide good time-average values. When the compound being measured is reactive, the initial values should not be used to assess an expected lifetime exposure. Instead, an effort should be made to calculate an average value. In addition, when the measured values are made near the source (i.e., in the air above contaminated soil or water) and the exposed population resides at some distance from this source, then the change in concentration attributable to atmospheric dispersion should be estimated.

Ground-water concentrations should be obtained from as many samples from as many wells as possible. An effort should be made to determine the distribution of concentrations within the public water supply connected to the contaminated wells. Dilution attributable to the distance of the well from the source and to blending with uncontaminated supplies should be assessed. Surface water concentrations should be measured in the water body closest to

the proximate source of either fish or drinking water. Soil and vegetation sources should be representative as possible of similar materials in private gardens, grazing lands, or food-crop fields.

Multimedia Simulations

It is often not practical or feasible to make appropriate measurements of environmental concentrations in air, soil, and water and to follow long-term changes in these concentrations. Thus, an exposure analyst may want to use numerical simulation to relate the source of contamination to time-varying environmental concentrations. In two companion reports, Layton et al. (1986) and McKone et al. (1987), and in the paper by McKone and Layton (1986), we describe the GEOTOX model that can be used to estimate environmental concentrations attributable to a steady-state or dynamic source of contaminants in air, water, and/or soil. Unlike media-specific models, this model simulates the simultaneous transport and transformation of chemicals among eight homogenous compartments that are used to represent the geographical region receiving the contaminants. When the exposed population is at some distance from the contaminated region, it is also necessary to account for the dilution of the estimated ground-water and atmospheric contaminant concentrations. In the following subsections we review relatively simple transport models that can be used in conjunction with the GEOTOX model to estimate contaminant transport to specific receptors. These models were chosen for the purpose of demonstrating their use in screening applications or preliminary assessments. Each of these models may be replaced with more sophisticated numerical and analytical models (e.g., finite-difference and finite-element models for ground water transport, Gaussian-diffusion models for atmospheric dispersion under differing climatic conditions, etc.), depending on the nature and needs of a site-specific exposure assessment.

Simple Dilution Models

As discussed above, there are situations in which the measured or simulated concentrations should be adjusted to account for the fact that the exposed population comes in contact with airborne or ground-water contaminants

at some distance from the source. In this subsection, we review some simple models that can be used to account for dilution in the atmosphere or ground-water zone.

Atmospheric dilution. If we assume that measured or simulated atmospheric-concentration measurements correspond to annual-average concentrations within an area that has a characteristic length s and a total distributed source Q, then we can use simple formulae proposed by Turner (1982) to estimate concentrations in adjacent landscapes.

According to Turner (1982, p. 38), for a constant source Q, the yearly average ground-level concentration at a distance r from a point source is

$$\chi = \frac{Q}{Lu\sigma_y(r)} \qquad (2\text{-}1)$$

where

χ = annual average ground level concentration, mg/m^3;
Q = annual average source term, mg/s;
L = annual average mixing height, m;
u = annual average wind speed, m/s;
$\sigma_y(r)$ = annual average standard deviation across the plume width, m; and
r = distance from the source, m.

Using 16 wind sectors, Turner (1982) shows that the standard deviation as a function of distance r in an arbitrarily selected sector is given by

$$\sigma_y(r) = \frac{2\pi r}{16} \qquad (2\text{-}2)$$

In dealing with the diffusion of contaminants when there are area sources, Turner (1982, p 39-40) states that the concentration within the source area is given by

$$\chi = \frac{Q}{Lu\sigma_{yo}} \qquad (2\text{-}3)$$

where σ_{yo} is the standard deviation at a virtual distance r_y that gives the appropriate concentration for the combined sources Q within the area. Using the virtual distance r_y, one can estimate the concentration at some distance r from the area source by treating the area source as an equivalent point source and calculating σ_y as a function of $r + r_y$. According to Turner (1982), the initial standard deviation of a square area source can be approximated by $\sigma_{yo} \cong s/4.3$, where s is the square root of source area, A. Combining this with equation 2-3, we obtain an expression for the air concentration within an area having contaminated soil emitting contaminants at an annual average rate of Q mg/s,

$$C_a = \frac{4.3\ Q}{Lu\sqrt{A}} \qquad (2\text{-}4)$$

where A is the size of the area enclosing the distributed sources and C_a corresponds to an air concentration measured in the contaminated area or obtained from GEOTOX. Combining the information above with equations 2-1 through 2-3 gives an expression for the concentration $C_a^*(r)$ at some distance r from the boundary of the area source:

$$C_a^*(r) = \frac{Q}{Lu\left[\frac{2\pi}{16}\, r + \frac{\sqrt{A}}{4.3}\right]} \quad . \qquad (2\text{-}5)$$

Combining equations 2-4 and 2-5 gives an expression for the concentration $C_a^*(r)$ at a distance r (in m) from a region with area A (in m^2) having a concentration C_a:

$$C_a^*(r) = C_a / \left(1.0 + 1.689\, \frac{r}{\sqrt{A}}\right) \quad . \qquad (2\text{-}6)$$

Ground-water dilution. In order to calculate dilution in ground water between the contaminated site and the point at which a well draws water from an aquifer, we use a model proposed by the U.S. EPA (1985). This model, referred to as the VHS model, was adapted by the U.S. EPA from a model proposed by Domenico and Palciauskas (1982). The model mathematically simulates the dilution of contaminant-bearing liquid in the ground water below the contaminated area.

Dilution occurs as a result of dispersion and transport within the aquifer. The VHS model is used to predict the maximum concentration of diluted contaminants at a compliance point 152 m from a hazardous waste site. For the current study, we use this model to estimate the dilution in the nearest well to a contaminated area where the contaminant concentration in the aquifer has been measured or estimated as C_g. The VHS equation expresses the ground-water concentration, $C_g^*(Y)$ at a distance Y from the contaminated area according to the expression,

$$C_g^*(Y) = C_g \text{ erf}\left[\left(\frac{Y'}{4Y}\right)^{1/2}\right] \times \text{erf}\left[\frac{X}{4\sqrt{(\alpha_t Y)}}\right] \qquad (2\text{-}7)$$

where

$C_g^*(Y)$ = ground-water concentration of a contaminant at a distance Y from the source area, mg/L;

Y = distance from the contaminated area to the reception point (i.e., the nearest well, the U.S. EPA recommends a value of 152.4 m for this parameter), m;

C_g = concentration of contaminant as measured or estimated within the ground-water zone of the area contaminated, mg/L;

erf( ) = error function defined as

$$\text{erf}(x) = (2/\sqrt{\pi}) \int_0^x \exp(-t^2)dt;$$

Y' = width of the contaminated area, m;

X = length of the contaminated area, m; and

α_t = transverse dispersivity within the aquifer, m [the U.S. EPA (1985) recommends a value of 2 m for this parameter].

The VHS model was developed by the U.S. EPA for establishing a reasonable worst-case disposal scenario for evaluating potentially hazardous waste sites. These evaluations enable the U.S. EPA to "examine the potential hazard of delisted wastes managed in non-hazardous-regulated disposal situations" (U.S. EPA, 1985). The model includes spreading or dispersion of contaminants

Table 2-1. Values of the dilution ratio $C_g^*(Y)/C_g$ as calculated using equation 2-7 for different areas.

Area, A in m^2	X,Y'= $\sqrt{A}$ in m	$C_g^*(Y)/C_g$
1,000	32	0.09
2,000	45	0.19
5,000	71	0.31
10,000	100	0.41
50,000	220	0.61
100,000	320	0.70
500,000	710	0.87
1,000,000	1,000	0.93

in the aquifer plume, but does not include retardation of a contaminant due to sorption. The U.S. EPA uses this model to predict the maximum concentration of the diluted contaminants at a compliance point located 500 ft (152.4 m) from the disposal site.

We assign Y' and X the value $X = Y' = \sqrt{A}$; where A is the area of the contaminated region, in m^2. Table 2-1 lists the ratio $C_g^*(Y)/C_g$ as a function of contaminated site area as calculated using Eq. 2-4, where, Y = 152.4 m, α_t = 2 m and $X = Y' = \sqrt{A}$.

EXPOSURE, DOSE, AND RISK

In this subsection, we define the concepts of exposure and dose in terms of human-health-risk assessments. The U.S. EPA (1987b) defines exposure as the contact with a physical or chemical agent. The measure of contact (environmental concentration or absorbed dose) depends upon how well we understand the relation between exposure, dose, and risk. An integrated exposure assessment quantifies this contact via all routes of exposure--inhalation, ingestion, and dermal--and all environmental media.

In order to comply with the U.S. EPA definition and to provide consistency with the concepts of exposure and dose as used for radioactive materials by the international scientific community (UNSCEAR, 1982; ICRP, 1977 and 1979), we provide both qualitative and quantitative definitions of exposure, dose, and risk:

Exposure expresses the amount of material or energy that is available at the human/environment exchange boundaries, which include the lung surfaces, gut wall, and skin surface. For a single event, exposure can be expressed as the total quantity (in mg) that comes in contact with the human system. For a continuous event, exposure can be expressed as either (a) the concentration of material (in mg/m^3) or (b) the rate at which a quantity of material (in mg/d or mg/d per kg body weight) comes in contact with the human system.†

Dose expresses the quantity of material or quantity of energy that is delivered to an organism or to a specific organ or tissue. For elements or chemicals, dose expresses either (a) the amount of material that crosses the human/environment exchange boundaries, in mg/kg-d; (b) the concentration of the species in blood, organs, or tissues, in mg/L or mg/kg; or (c) the amount of chemical metabolized, in mg/kg-d.†

Risk expresses the probability of detriment per individual or within a population, based on the distribution of dose within that population.

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† For exposure to radiations (both ionizing and non-ionizing); exposure expresses, for a single event, the quantity (in Bq) or the energy (in eV or J) that contacts the human system and, for a continuous event, the equivalent concentration (in Bq/m^3), the energy density (eV/m^3 or J/m^3), or the rate (in Bq/d, eV/s, or J/s) that radiation comes in contact with the human organism. For radiation, dose describes the deposition of energy (in J/kg) in an organism, organ, or tissue.

In general, we can say that the expected number of health effects, H, within a population of size N at a given dose level is related to a dose-response function Q,

$$H = Q(D)\ D(e_h, e_g, e_d)\ N \qquad (2\text{-}8)$$

where

H = number of health effects within a population of N people receiving the population-averaged dose D;

Q(D) = dose-response function that expresses the lifetime probability of detriment associated with the dose D, $(mg/kg\text{-}d)^{-1}$;

$D(e_h, e_g, e_d)$ = dose level associated with exposures e_h, e_g, e_d, mg/kg-d;

e_h = inhalation exposure, mg/kg-d;

e_g = ingestion exposure, mg/kg-d;

e_d = dermal contact, mg/kg-d; and

N = number of people within the exposed population.

Because there is uncertainty about levels of exposure, about the dose associated with any exposure, and about the dose-response function, it is often appropriate to employ a stochastic approach for estimating health effects within a population. As a result, this report presents ranges of values for parameters used to calculate exposure, and, where possible, provides the standard deviation associated with each parameter.

ANATOMICAL AND DIETARY PARAMETERS

Human exposure estimates are structured to provide input to a risk assessment. To achieve this, one must determine the lifetime-average exposure within the population in terms of the daily contact per unit body weight. This subsection reviews the anatomical and dietary parameters required for exposure estimates and provide tables of representative parameter values for children and adult males and females.

The dietary values presented here do not take into account fractions of the diet which are obtained from a contaminated region as opposed to those which are not. In terms of a preliminary analysis, it is assumed that all foodstuffs are obtained from the contaminated region. In terms of a detailed site-specific assessment, these fractions will have to be factored into analyses, but this is beyond the scope of this document.

Body Mass and Surface Area

Table 2-2 lists values of human body mass as a function of age and sex. The lower portion of this table lists values that are used in this report to characterize children, adult males, adult females, and the combined adult average. Values listed include both the arithmetic mean and the standard deviation. The mean and standard deviation for body mass listed in the upper portion of the table are taken directly from ICRP (1975). The child mass listed in the lower portion of the table is the age-weighted average mass and the standard deviation is the square root of the age-weighted sum of the variances in body mass. Both values are obtained from data over the age range from newborn to 15 years. The adult data for body mass and its standard deviation are based on the age range from 15 years to 70 years.

The surface area is calculated as a function of body weight using a formula taken from ICRP (1975),

$$SA = \frac{4W + 7}{W + 90} \qquad (2\text{-}9)$$

where

SA = surface area, m^2, and

W = body weight, kg.

The standard deviation in the surface area is calculated as the product of the derivative of surface area with respect to body weight (W) and the standard deviation in body weight,

$$\sigma_{SA} = \left[\frac{4}{W + 90} - \frac{4W + 7}{(W + 90)^2}\right] \sigma_W \quad . \qquad (2\text{-}10)$$

Table 2-2. Human body weight and surface area by age and sex (derived from ICRP, 1975).

Ages (y)	Sex	Mass (kg)[a]	Surface area[a] (m^2)
Newborn - 1	male/female	6.8 ± 2	0.35 ± 0.07
1 - 3	male/female	12 ± 2	0.54 ± 0.07
3 - 5	male/female	18 ± 2	0.73 ± 0.06
5 - 7	male/female	22 ± 2	0.85 ± 0.06
7 - 9	male/female	26 ± 5	0.96 ± 0.1
9 - 11	male/female	32 ± 5	1.1 ± 0.1
11 - 13	male/female	41 ± 8	1.3 ± 0.2
13 - 15	male/female	50 ± 8	1.5 ± 0.1
15 - 20	male	62 ± 8	1.6 ± 0.1
	female	55 ± 8	1.6 ± 0.1
20 - 40	male	70 ± 10	1.8 ± 0.1
	female	58 ± 9	1.6 ± 0.1
40 - 70	male	75 ± 10	1.9 ± 0.1
	female	62 ± 10	1.7 ± 0.2
Child Newborn to 15 y average	male/female	27 ± 14	0.95 ± 0.35
Adult 15 to 70 y average	male	72 ± 10	1.8 ± 0.1
	female	60 ± 10	1.6 ± 0.2
Adult combined average	male/female	66 ± 14	1.7 ± 0.2

[a] Arithmetic mean ± one standard deviation.

Breathing Rates

Table 2-3 lists breathing rates for children, adult males and females, and the average adult. These values are also derived from information in ICRP Report 23 (ICRP, 1975) and represent the arithmetic mean ± one standard deviation. For each age and sex category, the breathing rate is expressed in

Table 2-3. Reference breathing rates for children and adults (derived from ICRP, 1975).[a]

	Breathing[b] rate L/min	Hours per day	Daily volume m^3/d	Breathing rate per unit body weight[c] $m^3/kg\text{-}h$
Child (10 y)				
active	13 ± 4	16	12 ± 4	0.030 ± 0.044
resting	4.8 ± 1	8	2.3 ± 0.5	0.011 ± 0.033
Adult male				
active	20 ± 6	16	19 ± 6	0.017 ± 0.005
resting	7.5 ± 1	8	3.6 ± 0.5	0.0060 ± 0.0007
Adult female				
active	19 ± 2	16	18 ± 2	0.019 ± 0.001
resting	6 ± 1	8	2.9 ± 0.5	0.0060 ± 0.0009
Adult combined				
active	19.5 ± 6	16	19 ± 6	0.018 ± 0.0052
resting	6.8 ± 1	8	3.3 ± 0.5	0.0060 ± 0.0006

[a] All values are given as arithmetic mean ± one standard deviation.

[b] The variances in measured breathing rates are based on only two data points for adult male and females. The relative variance in child breathing rates is assumed to equal that of an adult male.

[c] In obtaining the variance in the ratio of breathing rate to body weight, covariance between the breathing rate and body weight is based on the assumption that breathing rate scales with body weight to the two thirds power. Although this assumption might be considered unrealistic, it should be noted that the variance in this ratio is dominated by variance in body mass and that this assumption provides a plausible upper bound on uncertainty.

terms of an individual's minute breathing rate in L/min, while active or resting; the number of active and resting hours; the daily volume of air (in m^3) taken in while an individual is active or resting; and the breathing rate per unit body weight in $m^3/kg\text{-}h$ while an individual is active or resting. We calculated the variance in the breathing rates for adult males and females based on two data points for these groups given in the ICRP (1975) report. There were no data in the ICRP report regarding the variance in child

breathing rates. Thus, we obtained a variance for the child by assuming the same relative variance in child breathing rates as that for adults. In obtaining the variance in the ratio of breathing rate to body weight, BR/W, we use a covariance between the breathing rate and body weight based on the assumption that breathing rate scales with body weight to the two thirds power. Under this assumption,

$$\sigma^2_{(BR/BW)} = \left(\frac{BR}{BW}\right)^2 \left[\left(\frac{\sigma_{BR}}{BR}\right)^2 + \left(\frac{\sigma_{BW}}{BW}\right)^2 - 2\sigma_{BR/BW}\right] \qquad (2\text{-}11)$$

where

$\sigma^2_{(BR/BW)}$ = variance in the ratio of breathing rate to body weight;
BR = breathing rate, m^3/h
BW = body weight, kg;
σ^2_{BR} = variance in the breathing rate;
σ^2_{BW} = variance in body weight; and
$\sigma_{BR/BW}$ = covariance between breathing rate and body weight.

Fluid Intake

Table 2-4 lists information and data used to calculate fluid intakes for children, adult females and males, and adults combined. The top portion of the tables lists the relative contributions to total fluid intake from tap water, milk, and other water-based drinks. This last category includes tea, coffee, soft drinks, beer, and other water-based beverages. This information is taken directly from the ICRP (1975) report. ICRP [illegible] 23 (ICRP, 1975) states that under normal conditions, adults consume between 1.0 to 2.4 L/d of fluids. We interpret this range as representing an average intake of 1.7 L/d with a standard deviation of 0.7 L/d. Under high environmental temperatures to 32°C, the report states that the daily adult fluid intake to be 3.3 L/d with a standard deviation of 0.9 L/d. The report also gives reference values for the daily intake of fluids by adult males, adult females, and children (age 10) as, respectively, 1.9, 1.4, and 1.4 L/d. This information was used to compile the values in Table 2-4. The fluid intake per unit body weight is calculated as the ratio of the mean fluid intake in each age/sex category to the mean body weight for that category. The variance in each ratio is

Table 2-4. Fluid intakes for children and adults (derived from ICRP, 1975).

	Child (10 y)	Adult female	Adult male	Adult combined
	Relative Contributions, %			
Tap water	14	7	8	7.5
Milk	32	14	15	14.5
Water-based drinks[a]	54	79	77	78
	L/d			
Fluid intake under normal conditions[b]	1.4 ± 0.6	1.4 ± 0.6	1.9 ± 0.8	1.7 ± 0.7
Fluid intake at high environmental temperatures[c]	2.7 ± 0.7	2.7 ± 0.7	3.8 ± 1	3.3 ± 0.9
	L/kg-d[d]			
Fluid intake per unit body weight				
Under normal conditions	0.05 ± 0.02	0.02 ± 0.01	0.03 ± 0.01	0.03 ± 0.01
At high environmental temperatures	0.10 ± 0.02	0.04 ± 0.01	0.05 ± 0.01	0.05 ± 0.01

[a] Includes tea, coffee, soft drinks, beer, and other beverages.

[b] Values presented are assumed to be arithmetic means ± one standard deviation. ICRP reports the range for adult combined intake and the assumed mean for the other categories. The bounds on this range are assumed to represent ± one SD and the resulting variance is scaled to the other values to obtain the appropriate standard deviations.

[c] ICRP only reports fluid intake and standard deviation at high environmental temperatures for the adult-combined intake. We obtained the other values by scaling the corresponding ratios of high-temperature intake to normal by the value of this ratio for adults combined.

[d] The variance in the ratio of fluid intake to body weight is calculated with a covariance between the fluid intake and body weight for each age/sex category that is based on the assumption that fluid intake scales with body weight to the two-thirds power. As was the case for breathing rates, this assumption provides an upper bound estimate of the variance in uptake per unit body weight. The variance in the ratio is dominated by body weight variance.

calculated under the assumption that the covariance between body weight and fluid intake for the reference age/sex categories can be estimated using the assumption that fluid intake scales with body weight to the two-thirds power. The combined variance is calculated as it was for the breathing rate to body weight ratio in Eq. 2-11.

It is of interest that some 30% of a child's and 15% of an adult's fluid intake consists of milk. Because we account for the intake of milk as a food intake, it appears that this amount should be excluded from the total fluid intake. Nonetheless, because of the uncertainty about daily intake of fluid per individual (standard deviation of ~ 40%) and because of the possibility that milk could be prepared using tap water, we elected to use total fluid intake as representative of the amount of fluid ingested from potable water supplies. Also, it should be noted that the biotransfer factors, which account for contaminant transfer from cattle intake to milk products, tend to account for the contaminants that transfer to the fat or mineral portion of milk and not necessarily the liquid portion (Travis and Arms, 1988; Kenaga, 1980).

Food Intake

In order to calculate food intakes, we used a recent set of data compiled by Yang and Nelson (1986). Yang and Nelson statistically analyzed data from the 1977-1978 USDA Nationwide Food Consumption Survey to estimate the daily intake of food by individuals in the general population of the United States. The National Food Consumption Survey used a stratified probability sample of households in the 48 conterminous states and the District of Columbia in each of four seasons from April 1977 through March 1978. The sample was designed to be representative of the United States. The samples were classified according to the geographic region of the country; geographic divisions within these regions; and central city, suburban, and nonmetropolitan populations. Data were collected for 30,770 individuals within 114 primary sampling units--indicating approximately 270 individuals per sampling unit.

Table 2-5 summarizes the results of the survey by Yang and Nelson (1986) for five food classes according to 10 age groups. For each food class and age group, this table provides a nation-wide average daily intake based on four seasons. The mean value of food intake is the mean of the means for the 114 sample units. The standard error represents the standard deviation of the

Table 2-5. Mean and standard error for the daily per caput intake from major food classes by age (taken from Yang and Nelson, 1986).

Age	Fraction of the population	Food intake by food class kg/d				
		Dairy products[a]	Meat[b]	Fish[c]	Fruits and vegetables[d]	Grains
0 to 1	0.014	0.569 ±0.034	0.0452 ±0.011	0.0009 ±0.0035	0.155 ±0.023	0.056 ±0.019
1 to 4	0.055	0.418 ±0.017	0.0923 ±0.0050	0.0068 ±0.0017	0.164 ±0.011	0.158 ±0.0094
5 to 9	0.069	0.493 ±0.014	0.128 ±0.0042	0.0109 ±0.0014	0.226 ±0.0094	0.216 ±0.0079
10 to 14	0.069	0.510 ±0.013	0.160 ±0.0039	0.0133 ±0.0013	0.262 ± 0088	0.248 ±0.0074
15 to 19	0.069	0.458 ±0.014	0.190 ±0.0042	0.0166 ±0.0014	0.266 ±0.0092	0.245 ±0.0078
20 to 24	0.068	0.308 ±0.018	0.195 ±0.0054	0.0187 ±0.0018	0.250 ±0.012	0.212 ±0.010
25 to 29	0.067	0.269 ±0.019	0.198 ±0.0055	0.0208 ±0.0019	0.272 ±0.012	0.215 ±0.010
30 to 39	0.13	0.237 ±0.015	0.201 ±0.0044	0.0195 ±0.0015	0.278 ±0.0097	0.202 ±0.0081
40 to 59	0.25	0.221 ±0.011	0.194 ±0.0034	0.0220 ±0.0011	0.316 ±0.0075	0.192 ±0.0063
60 and over	0.21	0.248 ±0.013	0.154 ±0.0038	0.0172 ±0.0013	0.331 ±0.0084	0.184 ±0.0071

[a] Dairy products include both milk and non-milk foods.

[b] Meat includes beef, pork, and other meats.

[c] Fish includes fin fish, shell fish, and other seafood.

[d] Fruits and vegetables include leafy vegetables, exposed produce, protected produce and other fruits and vegetables not covered in the categories just mentioned.

sample means among the primary sample units. Also given in Table 2-5 is the estimated fraction of the population in each age group. This information is also taken from Yang and Nelson (1986).

Dairy products include both milk and non-milk dairy products. According to Yang and Nelson (1986), 82% of the total dairy product intake consists of fresh cow's milk and the remainder consists of dry milk, butter, cheese, etc. Meat includes beef, pork, poultry, and other meats. Yang and Nelson report the respective breakdown of the daily meat intake as beef (51%), pork (16%), poultry (18%), and other meats (15%). Fish as a food class includes fin fish, shell fish, and other seafood. The food class fruits and vegetables includes leafy vegetables, such as cabbage, cauliflower, broccoli, celery, lettuce, and spinach; exposed produce, such as apples, pears, berries, cucumber, squash, grapes, peaches, tomatoes, string beans, etc.; protected produce such as carrots, beets, turnups, potatoes, legumes, melons, citrus fruits, etc.; and other vegetables, fruits, and mixtures of vegetables or fruits not covered in the above categories. According to Yang and Nelson (1986), the respective contributions to the total U.S. average diet are leafy vegetables, 14%; exposed produce, 30%; protected produce, 53%; and other produce, 3%.

Table 2-6 lists food intakes for children (ages 0 to 15) and adults (ages 15 to 70) derived from the data of Yang and Nelson (1986). For each age category and food class the intake value is the weighted average over the corresponding age groups in Table 2-5. The fraction of the population in each age group is used as a weighting factor. The standard error, which represents the standard deviation among the means of the 114 primary sample units, is converted to the standard deviation of the entire age category by multiplying the standard error by the square root of N, the number of people in each sample unit. According to Yang and Nelson, of the 270 people in each sample unit, 20.3% are in the age range 0 to 15 and the remainder are in the 15 to 70 age range.

The comparative range in Table 2-6 lists the range of values for intake by food class published by the ICRP (1975) and in Regulatory Guide 1.109 (U.S. NRC, 1977). The lower value in the range expresses "typical" values recommended in these publications; the upper values represents values suggested to calculate maximum annual average exposures. The last column in Table 2-6 gives the ratio of intake to body weight for each food class and age group. This ratio is obtained by dividing the mean food intake for the child

Table 2-6. Food intakes for children and adults (derived from Yang and Nelson, 1986).

Food type	Intake[a] (kg/d)	Standard error[b] (kg/d)	Standard deviation[c] (kg/d)	Comparative range[d] (kg/d)	Intake per unit body weight[e] (kg/kg-d)
		Child (0 to 15 y)			Mean, StdDev
Dairy products[f]	0.48	0.03	0.2	--	0.018, 0.005
Milk	0.39	0.03	0.2	0.47 to 0.9	0.014, 0.006
Meat	0.12	0.007	0.05	0.10 to 0.11	0.0044, 0.001
Fish	0.01	0.0007	0.005	0.021 to 0.071	0.00037, 0.0001
Fruits and vegetables	0.22	0.02	0.2	0.42 to 1.1	0.0080, 0.005
Grains	0.200	0.01	0.1	0.13 to 0.34	0.0074, 0.003
		Adult (15 to 70 y)			
Dairy products[f]	0.26	0.006	0.09	--	0.0040, 0.001
Milk	0.22	0.005	0.08	0.30 to 0.85	0.0033, 0.001
Meat	0.19	0.006	0.09	0.21 to 0.30	0.0028, 0.001
Fish	0.020	0.0007	0.01	0.021 to 0.071	0.00030, 0.0001
Fruits and vegetables	0.30	0.01	0.2	0.40 to 1.1	0.0045, 0.003
Grains	0.20	0.007	0.1	0.12 to 0.34	0.0030, 0.002

[a] All values are fresh mass.

[b] Based on the standard deviation among the means of 114 sample units used by Yang and Nelson (1986).

[c] Obtained from the standard error under the assumption that there are 214 adults and 56 children in each of the 114 sample units.

[d] The comparative range of values listed here reflects the range of values published in ICRP report 23 (ICRP, 1975) and in Regulatory guide 1.109 (U.S. NRC, 1977). The lower values expresses the "typical value"; the upper values represents that used to calculate maximum annual average exposures. Because of the different bases upon which estimates are made, the comparative range does not necessarily include the intake value.

[e] The intake per unit body weight is obtained by dividing the value in the first column by 27 kg for children and 66 kg for adults. The uncertainty range is ± one standard deviation. The variance in this ratio is obtained using a covariance between food intake and body weight derived from the assumption that food intake scales with body weight to the two-thirds power.

[f] Intake of dairy products includes milk.

and adult age categories by the mean body weight for these age categories. The variance, and thus the standard deviation, in each ratio is calculated under the assumption that covariance between body weight and food intake can be estimated by assuming that food intake scales with body weight to the two-thirds power. The combined variance is calculated as it was for the breathing-rate-to-body-weight and fluid-intake-to-body-weight ratios using Eq. 2-11. Although this assumption may appear unrealistic and seem to force an overestimate of the variance, it should be noted that the variance in this ratio is dominated by the variance in body weight.

PROPERTIES OF CATTLE

In order to calculate human exposures to chemicals in milk and meat it is important to have estimates of the inhalation and ingestion rates for both beef and dairy cows. Table 2-7 lists properties of cows that were obtained from a review of papers that addressed the transfer of contaminants from air, water, vegetation, or soil to beef and/or dairy cows.

Table 2-7. Beef and dairy cattle intakes used in the exposure assessment.

Intake	Beef Cattle	Dairy Cattle	Reference
Vegetation, intake (kg dry mass per day)	8.0	16.0	a
	--	12.0	b
	9.2	17.0	c
	15.0	15.0	d
	6.1	25.0	e
	6.1	25.0	e
	13.2	16.4	f
	16.5	16.5	g
	17.5	17.5	h
Arithmetic mean ± 1 StdDev	12 ± 4.4	17 ± 3.7	
Water intake (L/d)	37.6	37.6	a
	45.4	45.4	i
	50.0	60.0	d
Arithmetic mean ±1 StdDev	44 ± 6.3	48 ± 11	
Inhalation (m^3/d)	85	85	h
	130	130	j
	150	150	h
Arithmetic mean ± 1 StdDev	122 ± 33	122 ± 33	
Soil Ingestion (kg/d)	0.1	0.1	a
	0.25	0.25	e,k
	--	0.48	b
	0.50	0.50	c
	0.72	0.72	g
Arithmetic mean ± 1 StdDev	0.39 ± 0.27	0.41 ± 0.24	

a Travis and Hattemer-Frey (1987)

b Simmonds and Linsley (1981)

c Whicker and Kirchner (1987)

d U.S. NRC (1977)

e Kercher and Anspaugh (1984)

f Boone et al. (1981)

g Small (1984)

h Zach (1985)

i Rosenblatt and Small (1981)

j Anspaugh et al. (1971)

k Smith (1977)

3. EXPOSURE PATHWAYS ASSOCIATED WITH CONTAMINATED OUTDOOR AIR

This section provides information needed to calculate inhalation and ingestion exposures attributable to gaseous or particulate contaminants in ambient-outdoor air. Figure 3-1 illustrates the pathways that are considered in this section. The concentrations C_a and C_p in mg/m^3 of the contaminant as a gas or attached to particles in air are the starting points for the exposure estimates. We develop pathway exposure factors, (PEFs) for the following pathways:

(1) air gases or particles/inhalation, F_{aa}, F_{pa};
(2) air gases or particles/biota/vegetables and fruits, F_{av}, F_{pv};
(3) air gases or particles/biota/grains, F_{ag}, F_{pg};
(4) air gases and particles/cattle/meat, F_{at}, F_{pt}; and
(5) air gases and particles/cattle/milk, F_{ak}, F_{pk}.

In order to develop these factors, the overall atmospheric concentration in mg/m^3 is divided into two components--first, the quantity of contaminant that is attached to particles in the air, C_p in mg/m^3, and second, the quantity of contaminant that is in gaseous form in the air, C_a in mg/m^3. Particulate contaminants are defined as inert dust (e.g. soil) particles which have absorbed a specific contaminant in contrast to a solid mass of pure contaminant. In this report, we show how to calculate "reference" PEFs, which are based on the mean values of inhalation and ingestion per unit body weight listed in Section 2. For those who wish to calculate an upper or lower bound estimate, it is possible to substitute other values for these ratios from Section 2 using the estimated standard deviations.

INHALATION EXPOSURES ATTRIBUTABLE TO CONTAMINATED AMBIENT AIR

Once one has estimated the concentrations of contaminant in the gaseous and solid phases of outdoor air, one can calculate the daily average exposure within a population using the expression

$$e_h^a \left(C_a, C_p\right) = F_{aa}C_a + F_{pa}C_p \qquad (3\text{-}1)$$

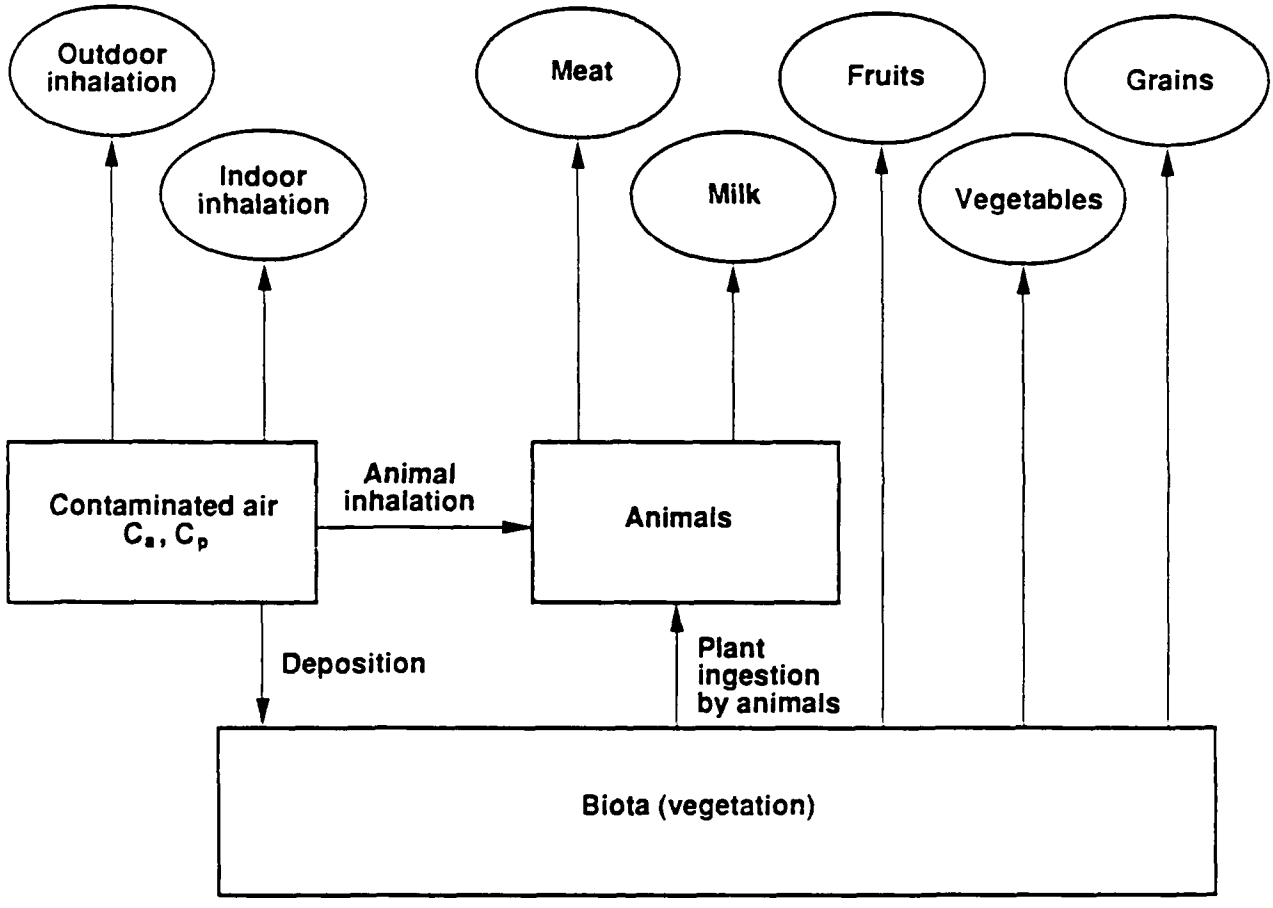

Figure 3-1. Exposure pathways originating from contaminated air, including deposition onto vegetation.

where

$e_h^a\left(C_a, C_p\right)$ = daily population exposure attributable to the contaminant concentrations C_a and C_p, mg/kg-d;

C_a = contaminant concentration in the gaseous phase of outdoor ambient air, mg/m^3;

C_p = contaminant concentration in the particulate phase of outdoor ambient air, mg/m^3; and

F_{aa}, F_{pa} = pathway exposure factors for, respectively, gas and solid phase contaminants in the outdoor ambient air, $(mg/kg\text{-}d)/(mg/m^3)$.

The pathway exposure factors F_{aa} and F_{pa} can be computed based on PEF's for adults and children, that is,

$$F_{aa} = \frac{15}{70} f_{aa}\left(\text{child}\right) + \frac{55}{70} f_{aa}\left(\text{adult}\right) \tag{3-2}$$

$$F_{pa} = \frac{15}{70} f_{pa}\left(\text{child}\right) + \frac{55}{70} f_{pa}\left(\text{adult}\right) \tag{3-3}$$

where $f_{aa}(child)$ and $f_{pa}(child)$ are PEF's for children and $f_{aa}(adult)$ and $f_{pa}(adult)$ are PEF's for adults. The factors 15/70 and 55/70 reflect the fraction of time an individual spends as a child and adult, respectively. We also use these numbers to estimate the fractions of a population that are children and adults. Another approach, which reflects the current age distribution in the U.S., would involve the use of age fractions reported in Yang and Nelson (1986) and listed in Table 2-5. However, this approach is not used here. The component PEF's are calculated as follows:

$$f_{pa}\left(\text{adult}\right) = 16\left[\frac{12}{16} \times 0.75 + \frac{4}{16}\right]\left(\frac{BR}{BW}\right)_a + 8 \times 0.75 \left(\frac{BR}{BW}\right)_r \tag{3-4}$$

$$f_{aa}\left(\text{adult}\right) = 16 \left(\frac{BR}{BW}\right)_a + 8 \left(\frac{BR}{BW}\right)_r \tag{3-5}$$

$$f_{pa}\left(\text{child}\right) = 16\left[\frac{12}{16} \times 0.75 + \frac{4}{16}\right]\left(\frac{BR}{BW}\right)_a + 8 \times 0.75 \left(\frac{BR}{BW}\right)_r \tag{3-6}$$

$$f_{aa}\left(\text{child}\right) = 16 \left(\frac{BR}{BW}\right)_a + 8 \left(\frac{BR}{BW}\right)_r \tag{3-7}$$

where

16 = number of hours per day that an adult or child is active;

8 = number of hours per day that an adult or child is resting;

12/16 = fraction of active hours that an adult or child spends indoors,

4/16 = fraction of active hours that an adult or child spends outdoors;

0.75 = level of suspended particulate matter indoors relative to that outdoors as reported by Hawley (1985);

$\left(\frac{BR}{BW}\right)_a$ = breathing rate per unit body weight for adults or children while active, based on Table 2-3, $(BR/BW)_a$ = 0.018 m^3/kg-h for adults and 0.030 m^3/kg-h for children; and

$\left(\frac{BR}{BW}\right)_r$ = breathing rate per unit body weight for adults or children while resting, based on Table 2-3, $(BR/BW)_r$ = 0.0060 m^3/kg-h for adults and 0.011 m^3/kg-h for children.

Substituting the appropriate values into Eqs. 3-4 through 3-7 gives:

$$f_{pa}\left(\text{adult}\right) = 16\left[0.813\right] \times 0.018 + 8 \times 0.75 \times 0.0060 = 0.27 \frac{(mg/kg\text{-}d)}{(mg/m^3)} ; \quad (3\text{-}8)$$

$$f_{aa}\left(\text{adult}\right) = 16 \times 0.018 + 8 \times 0.0060 = 0.34 \frac{(mg/kg\text{-}d)}{(mg/m^3)} ; \quad (3\text{-}9)$$

$$f_{pa}\left(\text{child}\right) = 16\left[0.813\right] \times 0.030 + 8 \times 0.75 \times 0.011$$

$$= 0.46 \frac{(mg/kg\text{-}d)}{(mg/m^3)} ; \text{ and} \quad (3\text{-}10)$$

$$f_{aa}\left(\text{child}\right) = 16 \times 0.030 + 8 \times 0.011 = 0.57 \frac{(mg/kg\text{-}d)}{(mg/m^3)} . \quad (3\text{-}11)$$

Substituting these values in Eqs. 3-2 and 3-3 gives:

$$F_{pa} = 0.31 \text{ (mg/kg-d)/(mg/m}^3\text{) and} \quad (3\text{-}12)$$

$$F_{aa} = 0.39 \text{ (mg/kg-d)/(mg/m}^3\text{)} . \quad (3\text{-}13)$$

FRUIT, VEGETABLE, AND GRAIN EXPOSURES ATTRIBUTABLE TO CONTAMINATED AMBIENT AIR

In calculating overall exposure, it is necessary to consider the transfer of small particles containing contaminants directly to the surface of vegetation. This transfer is not accounted for by plant/soil partition coefficients K_{sp} used in Layton et al. (1986) and McKone and Layton (1986). The pathway exposure factors F_{pv} and F_{pg} account for the ingestion of contaminants as a result of deposition from atmospheric particles to fruits, vegetables and grains. Similarly, contaminants that exist in gaseous form in the lower atmosphere can interact with the surfaces of fruits, vegetables, and grains through deposition processes. The ingestion exposure $e^a_{vg}(C_p, C_a)$ attributable to the concentration in mg/m^3 of contaminants in the solid phase C_p, and gas phase, C_a, of the atmosphere is given by the expression:

$$e^a_{vg}(C_p, C_a) = (F_{pv} + F_{pg})\, C_p + (F_{av} + F_{ag})\, C_a \qquad (3\text{-}14)$$

In this subsection, we develop expressions for the lifetime equivalent PEF's, F_{av}, F_{pv}, F_{ag}, and F_{pg}. Each is composed of the weighted sum of the child and adult PEF's. For example, the PEF for vegetable and fruit ingestion and attributable to atmospheric particles is given by,

$$F_{pv} = \frac{15}{70} f_{pv}\,(\text{child}) + \frac{55}{70} f_{pv}\,(\text{adult}) \qquad (3\text{-}15)$$

In order to calculate the transfer of atmospheric gases and particles from atmosphere to fruits, vegetables, and grains; we consider the balance between material that deposits on the exposed and edible portion of food crops and material that is removed by weathering and senescence. Using this model the PEFs for food crops are given by the following expressions:

$$F_{av} = \left[\frac{15}{70}\left(\frac{I_v}{BW}\right)_c + \frac{55}{70}\left(\frac{I_v}{BW}\right)_a\right] \times 0.47\, V_{da}\, f_v/(M_f R_v) \qquad (3\text{-}16)$$

$$F_{pv} = \left[\frac{15}{70}\left(\frac{I_v}{BW}\right)_c + \frac{55}{70}\left(\frac{I_v}{BW}\right)_a\right] \times 0.47\, V_{dp}\, f_v/(M_f R_v) \qquad (3\text{-}17)$$

$$F_{ag} = \left[\frac{15}{70}\left(\frac{I_g}{BW}\right)_c + \frac{55}{70}\left(\frac{I_g}{BW}\right)_a\right] \times V_{da}\ f_g/(M_f R_v) \quad (3\text{-}18)$$

$$F_{pg} = \left[\frac{15}{70}\left(\frac{I_g}{BW}\right)_c + \frac{55}{70}\left(\frac{I_g}{BW}\right)_a\right] \times V_{dp}\ f_g/(M_f R_v) \quad (3\text{-}19)$$

where,

15/70 = fraction of the population assumed to be children;

55/70 = fraction of the population assumed to be adults;

$\left(\frac{I_v}{BW}\right)_c$ = intake of vegetables and fruits per unit body weight for children as given in Table 2-6, 0.0080 kg (fresh mass)/kg-d;

$\left(\frac{I_v}{BW}\right)_a$ = intake of vegetables and fruits per unit body weight for adults as given in Table 2-6, 0.0045 kg (fresh mass)/kg-d;

$\left(\frac{I_g}{BW}\right)_c$ = intake of grains per unit body weight for children as given in Table 2-6, 0.0074 kg (fresh mass)/kg-d;

$\left(\frac{I_g}{BW}\right)_a$ = intake of grains per unit body weight for adults as given in Table 2-6, 0.0030 kg (fresh mass)/kg-d;

0.47 = fraction of the total mass of ingested fruits and vegetables that consists of unprotected produce or leafy vegetables;

V_{da} = deposition factor for the transfer of contaminant gas molecules to food crops, m/d;

V_{dp} = deposition factor for the transfer of atmospheric particles to food crops, m/d;

f_v = fraction of the target population's vegetables and fruits that come from the area with atmospheric concentrations C_a and C_p;

f_g = fraction of the target population's grains that come from the area with atmospheric concentrations C_a and C_p;

- M_f = annual average inventory of food crops per unit area, kg (fresh mass)/m^2; and

R_v = rate constant for the removal of chemicals from vegetation surfaces as a result of weathering and senescence, day^{-1}.

The deposition factors V_{da} and V_{dp} are the ratio of deposition rate on vegetation surfaces (in mg/m^2-d) to the air concentration in mg/m^3. These factors include both wet and dry deposition rates. Deposition rates and the resulting deposition factors are influenced by numerous factors and there are a wide range of reported values, for example from 3 to 4900 m/d reported for deposition rates from air to vegetation surfaces (Whicker and Kirchner, 1987). Shroeder and Lane (1988) report that dry deposition velocities measured for gases span four orders of magnitude from 0.002 cm/s (1.7 m/d) to 26 cm/s (22,000 m/d). They report deposition velocities measured for particles in the range from 0.001 cm/s (0.86 m/d) to 180 cm/s (155,000 m/d). McMahon and Denison (1979) report that, for particles less than 2 to 5 μm, dry deposition velocities to grasses and vegetation have been measured and range from 0.01 to 10 cm/s (8.64 to 8640 m/d).

Wet deposition processes have received much attention since it was discovered that they accounted for 80 to 90% of the total fallout from stratospheric nuclear weapons testing compared to 10 to 20% from dry deposition (Schroeder and Lane, 1988). Wet deposition involves the attachment of airborne pollutants to condensed atmospheric water--clouds, rain, or snow--either within or below a cloud. The efficiency with which wet deposition removes material from the atmosphere is assessed using the wash-out ratio, the ratio of contaminant concentration in air (mg/m^3) to contaminant concentration in precipitation (mg/m^3). According to Schroeder and Lane (1988), published experimental data indicate that the washout coefficient is about 2×10^5 for pollutants occuring primarily in the particulate phase of the atmosphere. With a yearly average rainfall of 1 m/y, this gives an equivalent total deposition velocity attributable to wet processes of 540 m/d. However, only a small fraction of this will be intercepted directly by vegetation surfaces.

Based on these observations, we estimate that deposition factors for gases to vegetation have an expected value of 600 m/d and a large variance (geometric standard deviation of about 4.5) and deposition factors for

particles <5 μm to vegetation surfaces have an expected value of 500 m/d and a geometric standard deviation of 3.0. The fractions f_v of fruits and vegetables and f_g of grains coming from contaminated areas are assumed to be 1.0. Whicker and Kirchner (1987) and Bowen (1979) report the inventory of standing and mature biomass, M_f, in agricultural landscapes to be on the order of 0.63 kg (dry mass)/m^2 or 3.0 kg (fresh mass)/m^2. The data reported in Layton et al. (1986) suggests that the variation in standing biomass is within a factor of three higher or lower than this value.

The work of Whicker and Kirchner (1987) provides data that allows one to estimate that for atmospheric particles the rate constant R_v is on the order of 0.03 day^{-1} with a range 0.01 to 1.0 day^{-1}. In the case of atmospheric gases, a representative value of the rate constant R_v is more difficult to estimate. In this case, we must recognize that removal of contaminants from vegetation surfaces can be caused by evaporation in addition to simple weathering processes and senescence. In order to estimate R_v for gases, we assume that the ratio of contaminant concentration in vegetation to that in surrounding air does not exceed the limits defined by chemical equilibrium and we adjust the value of R_v so that this ratio is not exceeded. From Eq. 3-16 and 3-18,

$$C_{vg} = V_{da}\, C_a/(M_f\, R_v) \qquad (3\text{-}20)$$

where C_{vg} is the contaminant concentration in fruits, vegetables, and grains in mg/kg (fresh mass). This simple relationship, of course, does not account for translocation within the plant.

We apply the restriction that

$$\frac{C_{vg}}{C_a} = \frac{RT}{H}\,(0.9 + 0.1\, K_{ow}) \times 10^{-3}\ m^3/L \qquad (3\text{-}21)$$

where R is the gas constant, 62.4 torr-L (air)/(mol-k), T is the ambient temperature, ~ 293K, H is the Henry's law constant with units torr-L/mol, and K_{ow} is the octanol/water partition coefficient. The conversion constant 10^{-3} adjusts the units on the right-hand side of Eq. 3-21 so that the units of C_a on the left-hand side are mg/m^3.

Equation 3-21 is constructed by assuming that the gas component of the air and the plant tissues have the same contaminant fugacity or partial pressure. For purposes of estimating fugacity we further assume that plant tissues are structured such that they can be modelled as containing 90% water and 10% organic material. (For more discussion about fugacity see Mackay (1979), Mackay and Paterson (1981), and Mackay and Paterson (198_).) Based on the assumptions just stated, the following relationships were developed and were used to derive Eq. 3-21.

- The ratio of the concentration of a contaminant in the water component of vegetation, C_{vg}^{w}, to the concentration of the contanimant in the gas component of air, C_a, is equal to $\frac{RT}{H}$;

- The concentration of a contaminant in the organic component of vegetation, C_{vg}^{o}, is equal to the product of C_{vg}^{w} multiplied by K_{ow}; and

- The total concentration of a contaminant in vegetation, C_{vg}, is equal to the sum of 0.9 x C_{vg}^{w} and 0.1 x C_{vg}^{o}.

Substituting Eq. 3-20 in Eq. 3-21 gives

$$R_v = \frac{V_{da}}{M_f} \times \frac{H}{RT} \times \frac{10^3}{(0.9 + 0.1\ K_{ow})} \qquad (3\text{-}22)$$

Making the appropriate substitutions in Eqs. 3-16 to 3-19 gives the following estimates for the mean values of the PEFs from gases and particles through vegetables and grains to humans:

$$F_{av} = 2.5 \times 10^{-6}\ (RT/H)(0.9 + 0.1\ K_{ow})\ (mg/kg\text{-}d)/(mg/m^3)\ , \qquad (3\text{-}23)$$

$$F_{pv} = 14\ (mg/kg\text{-}d)/(mg/m^3)\ , \qquad (3\text{-}24)$$

$$F_{ag} = 3.9 \times 10^{-6}\ (RT/H)(0.9 + 0.1\ K_{ow})\ (mg/kg\text{-}d)/(mg/m^3)\ , \text{ and} \qquad (3\text{-}25)$$

$$F_{pg} = 22\ (mg/kg\text{-}d)/(mg/m^3)\ . \qquad (3\text{-}26)$$

MILK AND MEAT EXPOSURES ATTRIBUTABLE TO CONTAMINATED AMBIENT AIR

This subsection explores how the concentration of a contaminant in the solid and gaseous phases of the atmosphere, C_p and C_a, can lead to contamination of meat and milk and thus result in human exposures. These exposures can be traced through two principal paths--the inhalation of atmospheric gases and particles by meat- and milk-producing cattle and the ingestion of contaminants deposited on the surfaces of vegetation consumed by these cattle. Once again the ingestion exposure for meat or milk is divided into two pathway exposure factors, one corresponding to atmospheric gases and one corresponding to atmospheric particles:

$$e_t^a(C_a, C_p) = F_{at}C_a + F_{pt}C_p \qquad (3\text{-}27)$$

$$e_k^a(C_a, C_p) = F_{ak}C_a + F_{pk}C_p \qquad (3\text{-}28)$$

where $e_t^a(C_a, C_p)$ and $e_k^a(C_a, C_p)$ represent the average daily exposure to meat and milk attributable to the atmospheric concentrations C_a of gases and C_p of particles (expressed in mg/m^3); F_{at} and F_{ak} are, respectively, the PEFs for meat and milk exposures attributable to gaseous contamination in the lower atmosphere; and F_{pt} and F_{pk} are the PEFs for meat and milk exposures attributable to particle contamination in the lower atmosphere. As in previous cases, the PEFs F_{at}, F_{ak}, F_{pt}, and F_{pk} can be decomposed into PEFs for adults and children, for example,

$$F_{at} = \frac{15}{70} f_{at}(\text{child}) + \frac{55}{70} f_{at}(\text{adult}) \quad . \qquad (3\text{-}29)$$

In general, the PEF for meat or dairy pathways is composed as follows:

PEF x atmospheric concentration = human intake of milk/meat x biotransfer factor x [inhalation uptake (cattle) + ingestion uptake (cattle)] x atmospheric concentration. (3-30)

Furthermore, the ingestion uptake by cattle equals the product of ingestion of vegetation by cattle and the contaminant concentration on the surfaces of pasture:

$$\text{ingestion uptake (cattle)} = \text{daily cattle ingestion} \times \text{pasture concentration} \qquad (3\text{-}31)$$

The pasture concentration is estimated as the steady-state concentration of contaminant on plant surfaces:

$$\text{pasture concentration} = \frac{\text{deposition factor} \times \text{air concentration}}{\text{crop inventory} \times \text{loss rates}} \qquad (3\text{-}32)$$

Based on these general relationships, the four PEFs in Eqs. 3-23 through 3-26 can be related to human ingestion of meat and dairy products, cattle properties, depostion factors, and meat and dairy biotransfer factors using the following expressions:

$$f_{at} = \frac{I_t}{BW} \left[I_{nc} + (I_{vbc} \; V_{da}) / (M_p R_v) \right] f_t \; B_t \qquad (3\text{-}33)$$

$$f_{pt} = \frac{I_t}{BW} \left[I_{nc} + (I_{vbc} \; V_{dp}) / (M_p R_v) \right] f_t \; B_t \qquad (3\text{-}34)$$

$$f_{ak} = \frac{I_k}{BW} \left[I_{nc} + (I_{vdc} \; V_{da}) / (M_p R_v) \right] f_k \; B_k \qquad (3\text{-}35)$$

$$f_{pk} = \frac{I_k}{BW} \left[I_{nc} + (I_{vdc} \; V_{dp}) / (M_p R_v) \right] f_k \; B_k \qquad (3\text{-}36)$$

where,

$\frac{I_t}{BW}$ = human intake per unit body weight of meat products, 0.0044 kg (fresh mass)/kg-d for children and 0.0028 kg (fresh mass)/kg-d for adults as listed in Table 2-6;

$\frac{I_k}{BW}$ = human intake per unit body weight of dairy products, 0.018 kg (fresh mass)/kg-d for children and 0.0040 kg (fresh-mass)/kg-d for adults as listed in Table 2-6;

I_{nc} = inhalation rate for beef and dairy cattle, 122 $\pm$ 33 m^3/d (Table 2-7);

I_{vbc} = ingestion rate of pasture grasses by beef cattle, 12 $\pm$ 4.4 kg (dry mass)/d (Table 2-7);

I_{vdc} = ingestion rate of pasture grasses by dairy cattle, 17 $\pm$ 3.7 kg (dry mass)/d (Table 2-7);

V_{da} = deposition factor for of contaminant gases from atmosphere to pasture surfaces, m/d;

V_{dp} = depostion factor for of contaminant particles (< 5 μm) from atmosphere to pasture surfaces, m/d;

M_p = the annual average inventory of pasture crops per unit area, kg (dry mass)/m^2;

R_v = Weathering and senecence rate constant, day^{-1};

f_t, f_k = respectively, the fractions of the target populations meat and dairy products that came from an area with contaminant concentrations, C_a and C_p;

B_t = biotransfer factor from cattle uptake to meat, the steady-state contaminant concentration in fresh meat divided by the animals' daily contaminant intake, (mg/kg)/(mg/d); and

B_k = biotransfer factor from cattle uptake to dairy products, the steady-state contaminant concentration in fresh dairy products divided by the daily contaminant intake by dairy cattle, (mg/kg)/(mg/d).

Values for the deposition factors, V_{da} and V_{dp} and the parameter R_v are assumed to be the same here as in the previous discussion on fruits, vegetables, and grains. The parameters f_t and f_k are both assigned the value

of unity. The density of dry mass pasture, M_p, is assumed to be on the order of 0.3 kg/m^2 with a likely range within a factor of ±3 (Whicker and Kirchner, 1987). The parameters B_t and B_k are dependent on the chemical form of the contaminant species. Methods for estimating B_t and B_k values and the variability in these values for the biotransfer factors are discussed in Appendix A.

Table 3-1 summarizes the expressions obtained for the age-specific PEFs when mean or median parameter values are substituted into Eqs. 3-33 through 3-36.

By combining the PEFs for children and adults and using the respective weighting factors 15/70 and 55/70, and applying the restriction that R_v = ([H/(RT)] x [10^3/(0.9 + 0.1 K_{ow})] x [V_{da}/M_p]) for gases as discussed in the previous subsection, we obtain the lifetime equivalent (or population average) PEFs for the meat and milk pathways. It should be noted that the parameter M_f in Eq. 3-22 is replaced here by the parameter M_p. This is done to reflect the fact that the milk and meat ingestion pathway model is based on the intake by cattle of dry pasture mass. Unlike fruits or vegetables the fugacity limit on plant concentration is here based on the dry mass inventory of pasture grasses.

$$F_{at} = [0.38 + 3.8 \times 10^{-4} (RT/H)(0.9 + 0.1 K_{ow})]B_t, \quad (3\text{-}37)$$

$$F_{pt} = 2100 B_t, \quad (3\text{-}38)$$

$$F_{ak} = [0.85 + 1.2 \times 10^{-3} (RT/H)(0.9 + 0.1 K_{ow})]B_k, \text{ and} \quad (3\text{-}39)$$

$$F_{pk} = 6600 B_k \quad . \quad (3\text{-}40)$$

Table 3-1. Age-specific PEFs for the air/meat and air/milk pathways.[a]

	Component PEF		
	Child	Adult	Combined child and adult PEF[b]
f_{at}	$[0.54 + 5.3 \times 10^{-4} (RT/H)(0.9 \times 0.1K_{ow})]B_t$	$[0.34 + 3.4 \times 10^{-4} (RT/H)(0.9 + 0.1K_{ow})]B_t$	$F_{at} = [0.38 + 3.8 \times 10^{-4}(RT/H)(0.9 + 0.1 K_{ow})]B_t$
f_{pt}	$2900 B_t$	$1900 B_t$	$F_{pt} = 2100 B_t$
f_{ak}	$2.2 + 3.1 \times 10^{-3} (RT/H)(0.9 + 0.1 K_{ow})]B_k$	$[0.49 + 6.8 \times 10^{-4}(RT/H)(0.9 + 0.1 K_{ow})]B_k$	$F_{ak} = [0.85 + 1.2 \times 10^{-3}(RT/H)(0.9 + 0.1 K_{ow})]B_k$
f_{pk}	$17,000 B_k$	$3800 B_k$	$F_{pk} = 6600 B_k$

[a] Units = $(mg/kg\text{-}d)/(mg/m^3)$

[b] Combined adult and child PEF = $\frac{15}{70}$ child PEF + $\frac{55}{70}$ adult PEF.

4. EXPOSURE PATHWAYS ASSOCIATED WITH CONTAMINATED SOIL

This section addresses procedures for calculating PEFs that relate contaminant exposure through inhalation, ingestion, and dermal absorption to contaminant concentrations in soil. Figure 4-1 illustrates the pathways that are addressed. The concentration in surface soil, C_s (in mg/kg), is the starting point for these exposure estimates. PEFs are estimated for the following pathways:

soil/indoor inhalation,
soil/fruits and vegetables,
soil/grains,
soil/pasture/cattle/meat,
soil/pasture/cattle/milk,
soil/soil ingestion, and,
soil/dermal absorption.

Following the procedure in Section 3, only "reference" PEFs are provided. Upper and lower bound values can be obtained by substituting alternate values for parameters used in this section and discussed here or in Section 2.

INDOOR INHALATION EXPOSURES ATTRIBUTABLE TO CONTAMINATED SOIL

House dust suspended in the indoor air environment may be thought of as originating from three sources, (1) airborne particulates that penetrate from outside air to indoor air; (2) surface soil and dust tracked into buildings on shoes or clothes, by pets, or other sources; and (3) a variety of sources related to occupant activities, material degradation, and household products. According to Murphy and Yocom (1986), several studies around smelters indicate that the second of these sources is the most important for exposure assessment. In this subsection, we develop a PEF that relates indoor air exposures from the second source to outdoor surface soil concentrations (C_s). We addressed the first source in Section 3 with the PEF that relates indoor inhalation exposures to contaminant concentrations of outdoor air particles (C_p). The third source is outside the scope of this report.

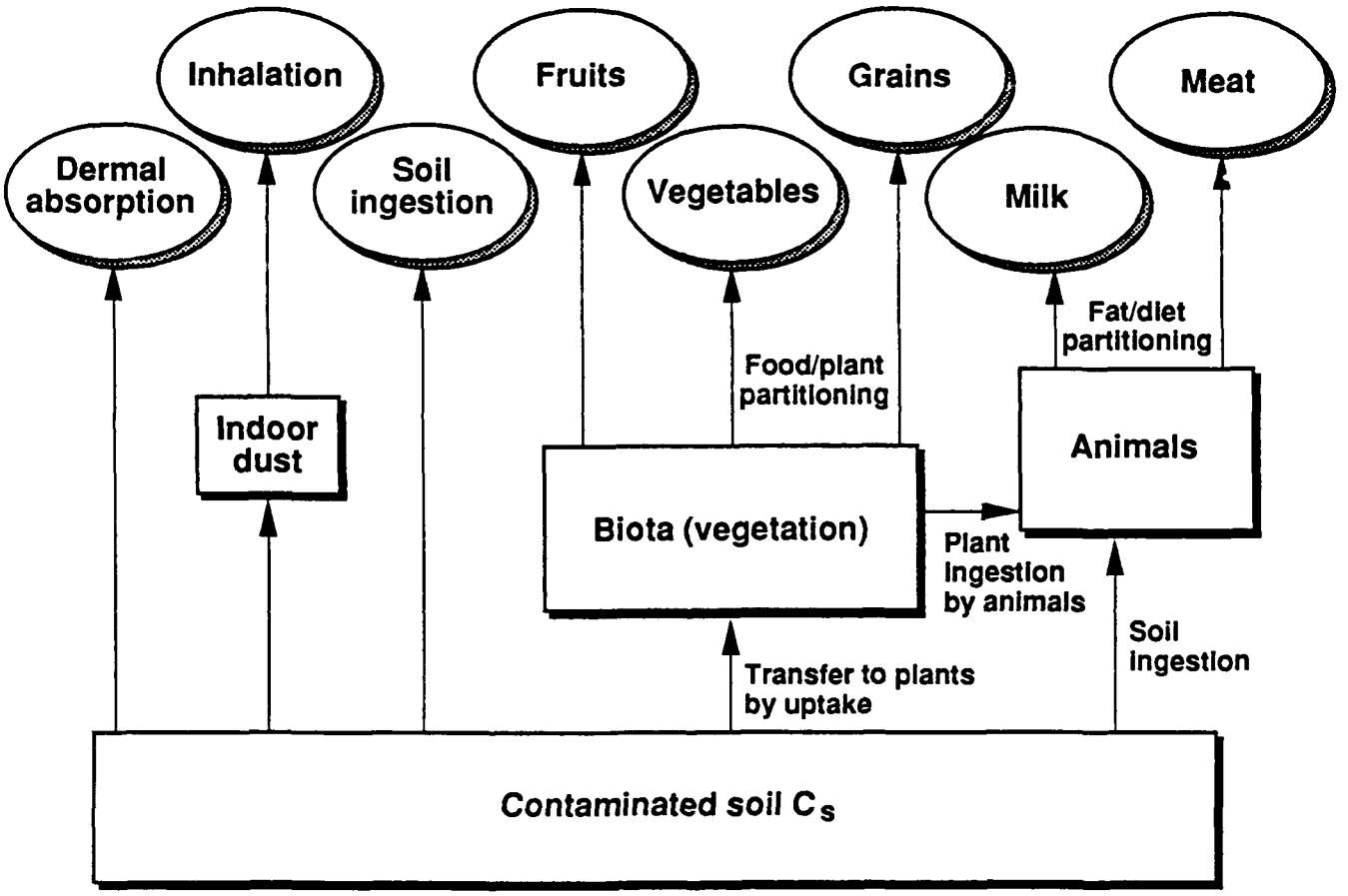

Figure 4-1. Soil-based exposure pathways for contaminants in surface soil.

Murphy and Yocom (1986) have estimated that the concentration of indoor particles that are attributable to surface soil is on the order of 30 $\mu g/m^3$ or 3.0×10^{-8} kg (soil)/m^3(air). Based on this value, and the assumption that both adults and children daily spend 4 out of 16 active hours outdoors, 12 out of 16 active hours indoors, and 8 out of 8 resting hours indoors, we have developed the following PEFs that relate indoor inhalation exposures to surface soil concentration:

$$f_{sa}\left(\begin{matrix}\text{adult or}\\ \text{child}\end{matrix}\right) = \left[16 \times \frac{12}{16}\left(\frac{BR}{BW}\right)_a + 8\left(\frac{BR}{BW}\right)_r\right] \times 3.0 \times 10^{-8} \text{ kg(soil)/m}^3\text{(air)} \qquad (4\text{-}1)$$

where

f_{sa} = pathway exposure factor (PEF) that converts outdoor soil concentration C_s to a daily indoor inhalation exposure, (mg/kg-d)/(mg/kg);

16 = number of hours per day that an adult or child is active;

12/16 = fraction of active hours that an adult or child spends indoors;

$(BR/BW)_a$ = the ratio of breathing rate to body weight while active, 0.018 (adult) and 0.030 (child) m^3/kg-h;

8 = number of hours per day that an adult or child is resting; and

$(BR/BW)_r$ = the ratio of breathing rate to body weight while resting, 0.006 (adult) and 0.011 (child) m^3/kg-h.

Making the appropriate substitutions gives

$$f_{sa}(\text{child}) = \left(16 \times \frac{12}{16} \times 0.030 + 8 \times 0.011\right) 3.0 \times 10^{-8}$$

$$= 1.3 \times 10^{-8} \text{ (mg/kg-d)/(mg/kg)} \qquad (4\text{-}2)$$

$$f_{sa}(\text{adult}) = \left(16 \times \frac{12}{16} \times 0.018 + 8 \times 0.0060\right) \times 3.0 \times 10^{-8}$$

$$= 7.9 \times 10^{-9} \text{ (mg/kg-d)/(mg/kg), and} \qquad (4\text{-}3)$$

$$F_{sa} = \frac{15}{70} f_{sa}(\text{child}) + \frac{55}{70} f_{sa}(\text{adult}) = 9.0 \times 10^{-9} \text{ (mg/kg-d)/(mg/kg)}. \qquad (4\text{-}4)$$

FRUIT, VEGETABLE, AND GRAIN EXPOSURES ATTRIBUTABLE TO CONTAMINATED SOIL

The PEF derived here accounts for the transfer of contaminants in soil to the internal portion of fruits, vegetables and grains. The concentrations C_b in the fresh mass of biota can be estimated using the plant/soil partition coefficient K_{sp},

$$C_b = 0.2 \times K_{sp} \times C_s \qquad (4\text{-}5)$$

where

C_b = concentration of contaminant per unit fresh mass of fruits, vegetables, and grains, mg/kg;

0.2 = dry mass fraction of fresh fruits, vegetables, and grains;

K_{sp} = plant soil partition coefficient, which expresses the contaminant concentration in biota dry mass per unit concentration in soil, [mg/kg(plant DM)]/[mg/kg(soil)]; and

C_s = contaminant concentration in soil, mg/kg.

Using Eq. 4-5, we derive the following expressions for the PEFs relating contaminant concentrations in fruits and vegetables or grains,

$$f_{sv}\left(\begin{matrix}\text{child or}\\ \text{adult}\end{matrix}\right) = 0.2\ K_{sp}\left(\frac{I_v}{BW}\right)\left(\begin{matrix}\text{child or}\\ \text{adult}\end{matrix}\right) \qquad (4\text{-}6)$$

$$f_{sg}\left(\begin{matrix}\text{child or}\\ \text{adult}\end{matrix}\right) = 0.2\ K_{sp}\left(\frac{I_g}{BW}\right)\left(\begin{matrix}\text{child or}\\ \text{adult}\end{matrix}\right) \qquad (4\text{-}7)$$

where f_{sv} is the PEF for contaminant transfer from soil to fruits and vegetables; f_{sg} is the PEF for soil to grain; and (I_v/BW) and (I_g/BW) express the intake, respectively, of fruits and vegetables or grains per unit body weight, kg/kg-d, for adults or children. Making the appropriate substitutions of the mean values for these parameters (see Table 2-6) gives:

$$\begin{aligned} f_{sv}(\text{child}) &= 0.2\ K_{sp} \times 0.0080\ \text{kg/kg-d} \\ &= 1.6 \times 10^{-3}\ K_{sp}\ \text{kg/kg-d or (mg/kg-d)/(mg/kg)} \end{aligned} \qquad (4\text{-}8)$$

$$f_{sg}(child) = 0.2\ K_{sp} \times 0.0074\ kg/kg\text{-}d \quad (4\text{-}9)$$
$$= 1.5 \times 10^{-3}\ K_{sp}\ (mg/kg\text{-}d)/(mg/kg)$$

$$f_{sv}(adult) = 0.2\ K_{sp} \times 0.0045\ kg/kg\text{-}d \quad (4\text{-}10)$$
$$= 9.0 \times 10^{-4}\ K_{sp}\ (mg/kg\text{-}d)/(mg/kg)$$

$$f_{sg}(adult) = 0.2\ K_{sp} \times 0.0030\ kg/kg\text{-}d \quad (4\text{-}12)$$
$$= 6.0 \times 10^{-4}\ (mg/kg\text{-}d)/(mg/kg)$$

As in previous sections, these numbers can be combined using the weighting factors 15/70 for children and 55/70 for adults and summing the results to give the population-equivalent PEFs,

$$F_{sv} = 1.1 \times 10^{-3}\ K_{sp}\ (mg/kg\text{-}d)/(mg/kg) \quad (4\text{-}13)$$

$$F_{sg} = 7.9 \times 10^{-4}\ K_{sp}\ (mg/kg\text{-}d)/(mg/kg) \quad (4\text{-}14)$$

MILK AND MEAT EXPOSURES ATTRIBUTABLE TO CONTAMINATED SOIL

Contaminants in surface soil can enter meat or milk through either the direct ingestion of soil by cattle or the ingestion by cattle of pasture grass that has taken up a contaminant from soil.

The PEFs, F_{st} and F_{sk} account for human contaminant exposures attributable to ingestion of contaminated soil and pasture vegetation by beef and dairy cattle. The expressions that link soil concentrations C_s and the PEFs to human exposure in mg/kg-d through meat, $e_t^s(C_s)$ and dairy products $e_k^s(C_s)$ are as follows:

$$e_t^s(C_s) = F_{st}\ C_s \quad (4\text{-}15)$$

$$e_k^s(C_s) = F_{sk}\ C_s \quad (4\text{-}16)$$

As in previous sections, the population-equivalent PEFs, F_{st} and F_{sk}, can be represented as the weighted combination of the child and adult age-specific component PEFs, f_{st} and f_{sk}:

$$F_{st} = 15/70\ f_{st}(child) + 55/70\ f_{st}(adult) \quad (4\text{-}17)$$

$$F_{sk} = 15/70\ f_{sk}(child) + 55/70\ f_{sk}(adult) \quad (4\text{-}18)$$

Following the protocol in Section 3, the PEF for meat and dairy pathways attributable to soil can be decomposed as follows:

$$\begin{aligned} \text{PEF} \times \text{soil concentration} &= \text{human intake of meat/milk} \\ &\times \text{biotransfer factor} \times \text{ingestion uptake (cattle)} \\ &\times \text{soil concentration} \end{aligned} \quad (4\text{-}19)$$

The ingestion uptake by cattle is composed of direct ingestion of soil contaminant and ingestion of contaminant that has been taken up from the soil into the edible plant parts.

Based on these conditions, the PEFs in Eqs. 4-17 and 4-18 can be calculated using the following expressions:

$$f_{st} = \left(\frac{I_t}{BW}\right) \times \left(I_{sc} + I_{vbc}\ K_{sp}\right) f_t\ B_t \quad (4\text{-}20)$$

$$f_{sk} = \left(\frac{I_k}{BW}\right) \times \left(I_{sc} + I_{vdc}\ K_{sp}\right) f_k\ B_k \quad (4\text{-}21)$$

where

$\left(\frac{I_t}{BW}\right)$ = human intake per unit body weight of meat, 0.0044 kg (fresh mass)/kg-d for children and 0.0028 kg (fresh mass)/kg-d for adults as listed in Table 2-6;

$\left(\frac{I_k}{BW}\right)$ = human intake per unit body weight of dairy products, 0.018 kg (fresh mass)/kg-d for children and 0.0040 kg (fresh mass)/kg-d for adults as listed in Table 2-6;

I_{sc} = soil ingestion rate for beef and dairy cattle, ~ 0.40 ± 0.25 kg/d as listed in Table 2-7;

I_{vbc} = ingestion rate of pasture grasses by beef cattle, 12 ± 4.4 kg (dry mass)/d (Table 2-7);

I_{vdc} = ingestion rate of pasture grasses by dairy cattle, 17 ± 3.7 kg (dry mass)/d (Table 2-7);

K_{sp} = plant/soil partition coefficient, mg/kg in edible plant parts (dry mass) divided by the mg/kg of contaminant in soil;

f_t, f_k = respectively, the fractions of the target population's meat and dairy products that come from an area with contaminant concentration, C_s, in soil; and

B_t, B_k = biotransfer factors for contaminant uptake to, respectively, meat and milk per unit intake by beef or dairy cattle, (mg/kg)/(mg/d).

Table 4-1 summarizes the expressions obtained for the age specific PEFs when mean (or median) values of the parameters are substituted into Eqs. 4-20 and 4-21. The parameters f_k and f_t are assumed to be 1.

Combining the PEFs for children and adults according to Eqs. 4-17 and 4-18 gives the population average (or lifetime equivalent) PEFs for the soil/meat and soil/milk pathways;

$$F_{st} = (0.0013 + 0.038\ K_{sp})\ B_t \qquad (4\text{-}22)$$

$$F_{sk} = (0.0028 + 0.12\ K_{sp})\ B_k \qquad (4\text{-}23)$$

Methods for calculating the biotransfer factors B_t and B_k are discussed in Appendix A.

SOIL INGESTION EXPOSURES

Assessing human exposures to contaminants in soil through direct ingestion of soil requires an estimate of age-dependent human soil ingestion.

Table 4-1. Age-specific component PEFs for the soil/meat and soil/milk pathways.[a]

	f_{st}	f_{sk}
child	$(0.0018 + 0.053\ K_{sp})\ B_t$	$(0.0072 + 0.31\ K_{sp})\ B_k$
adult	$(0.0011 + 0.034\ K_{sp})\ B_t$	$(0.0016 + 0.068\ K_{sp})\ B_k$

[a] Units = (mg/kg-d)/(mg/kg)

LaGoy (1987) has reviewed empirical data on human soil ingestion and used these data to make preliminary estimates of human soil ingestion rates for use in risk assessment. Table 4-2 summarizes LaGoy's preliminary findings.

Using the numbers in Table 4-2, we calculate the average intake of soil by a child 0 to 11 y to be 4.3 mg/kg-d and use this value to represent children in the range of 0 to 15 y. We use average daily intake of soil by individuals 11 to 70 years of age as the representative value for adults. Listed below are the age-specific PEFs for soil ingestion that we have derived using the information in Table 4-2 and a factor of 10^{-6} that relates mg of soil to kg of soil.

$$f_{ss}(\text{child}) = 4.3 \times 10^{-6}(\text{mg/kg-d})/(\text{mg/kg}) \qquad (4\text{-}24)$$

$$f_{ss}(\text{adult}) = 7.1 \times 10^{-7}(\text{mg/kg-d})/(\text{mg/kg}) \qquad (4\text{-}25)$$

The population PEF is calculated as the weighted sum of the two age-specific terms:

$$F_{ss} = \frac{15}{70} f_{ss}(\text{child}) + \frac{55}{70} f_{ss}(\text{adult})$$

$$= 1.5 \times 10^{-6}(\text{mg/kg-d})/(\text{mg/kg}) \quad . \qquad (4\text{-}26)$$

DERMAL ABSORPTION EXPOSURES FROM CONTAMINATED SOIL

Dermal absorption of contaminants from soil occurs through the accumulation of contaminated soil on skin. The amount of soil that accumulates on human skin depends on a number of factors such as age, type of soil, exposed surface area, soil conditions, etc. There is a great deal of

Table 4-2. Estimates of soil ingestion rates, based on LaGoy (1987).

Age (y)	Average weight (kg)	Maximum intake[a] mg/d	Average intake mg/d	Average intake mg/kg-d
0-1	10	250	50	5.0
1-6	15	500	100	6.7
6-11	30	250	50	1.7
11-70	70	100	50[b]	0.71

[a] This does not include individuals who exhibit pica, for these individuals, LaGoy (1987) suggests a maximum intake of 5,000 mg/d.

[b] This value represents adults who engage in outdoor activities or exhibit frequent hand to mouth contact.

variability in these factors, making the estimation of soil dermal absorption a relatively uncertain process. In order to calculate a PEF for dermal absorption from soil, we define the exposure for this pathway in terms of the amount of soil contaminant that passes from the soil matrix on the skin into the underlying tissue. Hawley (1985) has reviewed the soil dermal-exposure pathway and made the following assumptions regarding this pathway:

- the absorption rates for pure compounds on the skin surface are on the order of 12% per day for adults and 24% per day for children;
- the duration of dermal absorption from soil is on the order of 12 h per day; and
- the absorption of compounds from a soil matrix is on the order of 15% of that for pure compounds.

We assume that the heads and upper extremities of both children and adults are the portions of the body that accumulate soil particles. According to the ICRP (1975), these components comprise 30% of the surface area of a child and 26% of the surface area of an adult. According to the data in Table 2-2 the

total surface area of a child is 0.95 m^2 and that of an adult is 1.7 m^2. Dividing these values by the respective body weights for these age groups gives the weight-specific surface area of children as 0.035 m^2/kg and of adults as 0.026 m^2/kg.

Lepow et al. (1975) have measured the concentration of soil on the hands of children and found an average of 0.005 kg/m^2. Roels et al. (1980) measured the amounts of lead on the hands of children relative to that in soil. Their work indicates that soil concentrations on the extremities of children are on the order of 0.05 kg/m^2. Based on these measurements, and the assumption that adults who work outdoors have the same soil concentration on their extremities as children, we assume that both adults and children have soil concentrations on their extremities of 0.03 kg/m^2. Combining the information above gives the following expressions and values for PEFs for soil dermal-absorption:

$$f_{sd}(\text{child}) = 0.30 \times 0.035\ m^2/kg \times 0.24/d \times 0.15 \times \frac{12\ h}{24\ h} \times 0.03\ kg/m^2$$

$$= 5.7 \times 10^{-6}\ (mg/kg\text{-}d)/(mg/kg) \quad , \qquad (4\text{-}27)$$

$$f_{sd}(\text{adult}) = 0.26 \times 0.026\ m^2/kg \times 0.12/d \times 0.15 \times \frac{12\ h}{24\ h} \times 0.03\ kg/m^2$$

$$= 1.8 \times 10^{-6}\ (mg/kg\text{-}d)/(mg/kg) \text{ , and} \qquad (4\text{-}28)$$

$$F_{sd} = \frac{15}{70} f_{sd}(\text{child}) + \frac{55}{70} f_{sd}(\text{adult}) = 2.6 \times 10^{-6}\ (mg/kg\text{-}d)/(mg/kg) \quad . \qquad (4\text{-}29)$$

5. EXPOSURE PATHWAYS ASSOCIATED WITH CONTAMINATED SURFACE AND GROUND WATER

This section provides procedures for calculating ingestion, inhalation, and dermal absorption exposures attributable to chemicals in ground and surface water. Figure 5-1 illustrates the pathways that are addressed. The concentrations C_r and C_g (in mg/L) of the contaminant in surface and ground water are starting points for these exposure estimates. PEFs are estimated for the following pathways:

surface water/fish,
potable water/drinking water intake,
potable water/inhalation,
potable water/dermal absorption,
surface or ground water/cattle/milk, and
surface or ground water/cattle/meat.

As in sections 3 and 4, only "reference" PEFs are calculated. Upper and lower bound values can be obtained by substituting alternate values for the parameters presented in this section.

SURFACE WATER CONTAMINATION AND FISH INGESTION EXPOSURES

In calculating the intake of contaminants by the fish pathway, we assume that fish and other seafood are in chemical equilibrium with surface waters so that the contaminant concentration in fish tissue C_f is equal to the surface water contaminant concentration C_r times the bioconcentration factor in fish BCF, or

$$C_f = BCF \times C_r \quad . \tag{5-1}$$

The daily average exposure attributable to the transfer of contaminants from water to fish is represented by the expression

$$e_f^r (C_r) = F_{rf} C_r \tag{5-2}$$

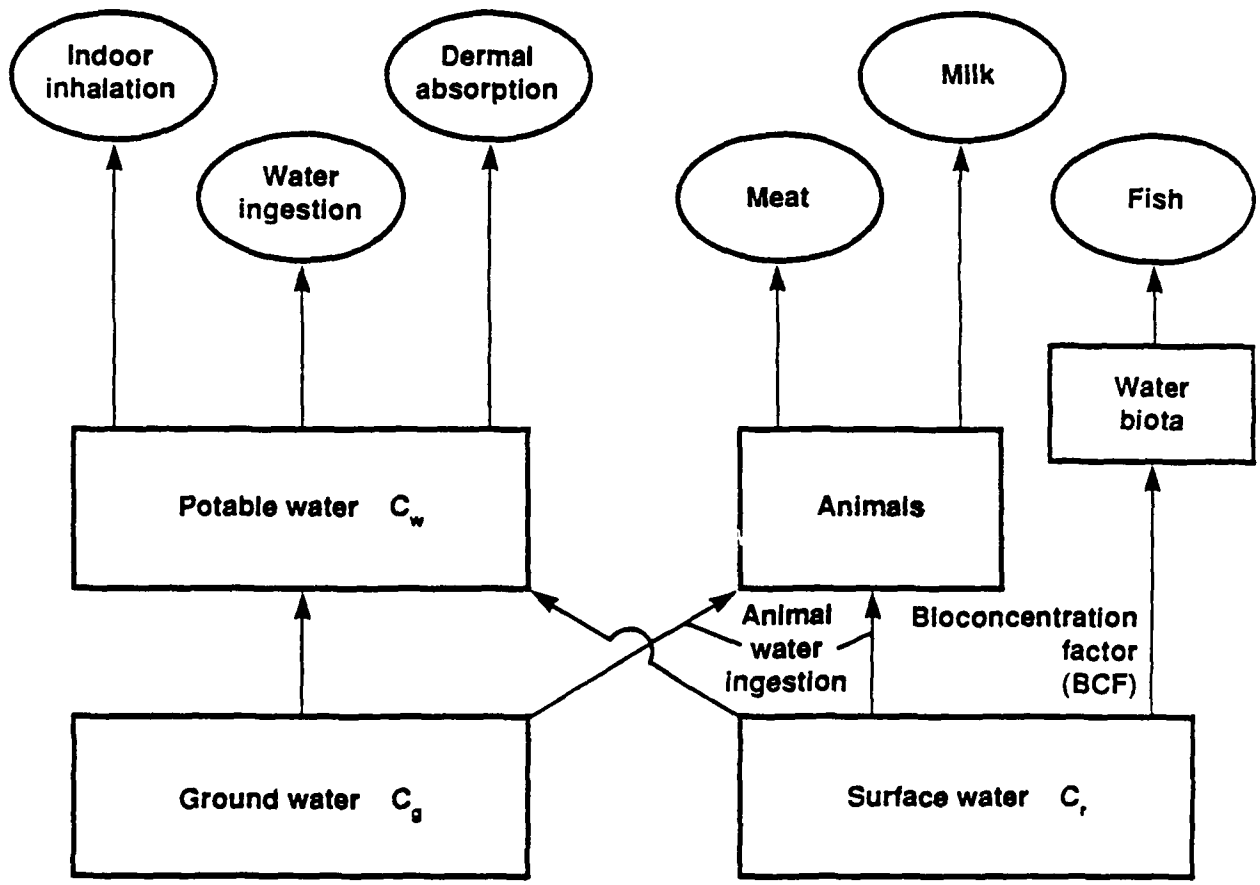

Figure 5-1. Water-based exposure pathways.

where

$$F_{rf} = \frac{15}{70} f_{rf}(\text{child}) + \frac{55}{70} f_{rf}(\text{adult}) \quad (5\text{-}3)$$

and where

$e_f^r (C_r)$ = daily population exposure through fish and seafood in mg/kg-d attributable to the surface-water concentration C_r, in mg/L;

F_{rf} = lifetime equivalent pathway exposure factor for fish ingestion, (mg/kg-d)/(mg/L); and

$f_{rf}\begin{pmatrix}\text{child or}\\ \text{adult}\end{pmatrix}$ = pathway exposure factors for a child or adult, (mg/kg-d)/(mg/L)

The daily intake of a contaminant through fish caught locally is the product of contaminant concentration in fish times the ingestion of fish per unit body weight per day. Based on this

$$f_{rf}(\text{child}) = \left(\frac{I_f}{BW}\right)_{\text{child}} \times \text{BCF} \quad (5\text{-}4)$$

$$f_{rf}(\text{child}) = \left(\frac{I_f}{BW}\right)_{\text{adult}} \times \text{BCF} \quad (5\text{-}5)$$

where $(I_f/BW)_{child}$ and $(I_f/BW)_{adult}$ are the daily intakes of fish per unit body weight of adults and children. Substituting parameter values from Table 2-6 gives

$$f_{rf}(\text{child}) = 0.00037 \text{ (kg/kg-d)} \times \text{BCF} \quad (5\text{-}6)$$

$$f_{rf}(\text{adult}) = 0.00030 \text{ (kg/kg-d)} \times \text{BCF} \quad (5\text{-}7)$$

and

$$F_{rf} = 0.00032 \text{ BCF (mg/kg-d)/(mg/L)}. \quad (5\text{-}8)$$

The factor BCF is assumed to have the units (mg/kg)/(mg/L).

EXPOSURE ATTRIBUTABLE TO DRINKING WATER INTAKE

For the water-ingestion pathway, the pathway exposure factor F_{ww} is used to convert the water supply concentration C_w (in mg/L) to a population equivalent exposure $e_w^w(C_w)$ (in mg/kg-d),

$$e_w^w(C_w) = F_{ww}C_w \qquad (5\text{-}8)$$

and

$$F_{ww} = \frac{15}{70} f_{ww}(\text{child}) + \frac{55}{70} f_{ww}(\text{adult}) \qquad (5\text{-}9)$$

The exposure factors f_{ww}(child) and f_{ww}(adult) are simply the ratio of water intake to body weight as listed in Table 2-4. And therefore, F_{ww} is computed as

$$F_{ww} = \frac{15}{70} \times 0.05 + \frac{55}{70} \times 0.03 \quad , \text{ or} \qquad (5\text{-}10)$$

$$F_{ww} = 0.034 \text{ (mg/kg-d)/(mg/L)} \quad . \qquad (5\text{-}11)$$

INHALATION EXPOSURES ATTRIBUTABLE TO POTABLE WATER

McKone (1987) has developed a model that describes the daily concentration profiles of volatile compounds within various compartments of the indoor air environment as a result of home water use. The results of this model provide a basis for calculating the pathway exposure factor, F_{wa}, that can be used to estimate the inhalation exposure $e_h^w\left(C_w\right)$ (in mg/kg-d) attributable to water supply contamination C_w (in mg/L)

$$e_h^w\left(C_w\right) = F_{wa} \times C_w \qquad (5\text{-}12)$$

where as before,

$$F_{wa} = \frac{15}{70} f_{wa}(\text{child}) + \frac{55}{70} f_{wa}(\text{adult}) \qquad (5\text{-}13)$$

in which f_{wa}(child) and f_{wa}(adult) are the component PEFs for adults and children.

The McKone (1987) model divides the indoor-air volume into three compartments--the shower/bath stall, the bathroom, and the remaining household volume. Concentrations within these compartments are dependent on chemical mass transfers from water to air, compartment volumes, and air-exchange rates. Using measured mass-transfer efficiencies from water to air for radon, McKone (1987) has estimated the typical or "reference" average concentrations of a chemical having the mass transfer efficiency of radon. These "reference" concentrations for the shower, C_{sh}, bathroom C_{ba}, and remaining house C_{ho} as calculated for radon with a concentration of 1 mg/L in water are summarized below.

C_{sh} = 27 mg/m^3 in shower air per mg/L in water during the period when showers are in use (the period from 7:00 to 8:00 a.m.),

C_{ba} = 7.3 mg/m^3 in bathroom air per mg/L in water during the period when the bathroom and shower are being used (the period from 7:00 to 9:00 a.m.),

C_{ho} (day) = 0.16 mg/m^3 in household air per mg/L in water during the day (from 7:00 a.m. to 11:00 p.m.), and

C_{ho} (night) = 0.035 mg/m^3 in household air per mg/L in water during the night (from 11:00 p.m. to 7:00 a.m.).

In addition, McKone (1987) shows that the concentration $C_x^j(t)$ in any household compartment for a compound j with a mass-transfer efficiency different from that of radon can be estimated from the expression,

$$C_x^j(t) = C_x^{Rn}(t) \times 2.0 \times 10^6 (m^2/s)^{-2/3} \left[2.5/D_\ell^{2/3} + RT/\left(D_a^{2/3} H\right) \right]^{-1} \qquad (5\text{-}14)$$

where

$C_x^j(t)$ = time-dependent concentration of a contaminant j in household compartment x, mg/m^3;

$C_x^{Rn}(t)$ = time-dependent concentration of a contaminant with the mass transfer properties of radon in household compartment x, mg/m^3;

D_ℓ = diffusion coefficient in water of contaminant j, m^2/s;
R = gas constant, 62.4 torr-L/mol-K;
T = temperature, kelvins;
D_a = diffusion coefficient in air of contaminant j, m^2/s; and
H = Henry's law constant, torr-L/mol.

For volatile substances, for which the Henry's law constant is large, the right-hand side of Eq. 5-14 becomes proportional to the water diffusion coefficient to the two-thirds power. In the case of a substance with a very low Henry's law constant, the right-hand side is proportional to the Henry's law constant.

Using a three-compartment model representing a reference house, McKone (1987) has shown that the daily inhalation exposure attributable to a water-supply concentration C_w is

$$E = \left(\frac{1}{BW} \int_0^{24h} \left[OF_{sh}(t)C_{sh}(t) + OF_{ba}(t)C_{ba}(t) + OF_{ho}(t)C_{ho}(t) \right] BR(t)\, dt \right) C_w \qquad (5\text{-}15)$$

where E is daily exposure, mg/kg-d, for an individual with body weight BW (in kg) and breathing-rate profile BR(t) (in m^3/h). $OF_{sh}(t)$, $OF_{ba}(t)$, and $OF_{ho}(t)$ are occupancy factors that express the probability that a given individual is in the shower, bathroom, or house at time t. McKone (1987) suggests that "reference" values for these parameters are respectively:

$OF_{sh}(t)$ = 10 min/60 min during the period 7:00 a.m. to 8:00 a.m. and zero otherwise,
$OF_{ba}(t)$ = 20 min/120 min during the period 7:00 a.m. to 9:00 a.m. and zero otherwise, and
$OF_{ho}(t)$ = 4 h/16 h during the period 7:00 a.m. to 11:00 p.m. and 8 h/8 h during the period 11:00 p.m. to 7:00 a.m.

It is assumed here that these values are valid for both children and adults. Substituting these values into Eq. 5-15 together with the average compartment concentrations discussed above gives:

$$E = \left[\left(27\ C_w \times 0.17 \times 1\ h + 7.3\ C_w \times 0.17 \times 2\ h + 0.16\ C_w \times 0.25 \times 16\ h\right) \frac{BR}{BW}\ (day) + 0.035\ C_w \times 8\ h \times \frac{BR}{BW}\ (night)\right] \times 2.00 \times 10^6\ (m^2/s)^{-2/3} \left[2.5/D_\ell^{2/3} + RT/\left(D_a^{2/3} H\right)\right]^{-1} mg/kg\text{-}d \qquad (5\text{-}16)$$

Dividing this expression by C_w and substituting the appropriate values of the ratios BR(day)/BW and BR(night)/BW from Table 2-3 provides sufficient information for calculating the exposure factors f_{wa}(child) and f_{wa}(adult). From Table 2-3 we obtain the following values for BR/BW:

$$\frac{BR}{BW}\ (day, adult) = 0.018\ m^3/kg\text{-}h\ , \qquad (5\text{-}17)$$

$$\frac{BR}{BW}\ (night, adult) = 0.0060\ m^3/kg\text{-}h\ , \qquad (5\text{-}18)$$

$$\frac{BR}{BW}\ (day, child) = 0.030\ m^3/kg\text{-}h, \text{ and} \qquad (5\text{-}19)$$

$$\frac{BR}{BW}\ (night, child) = 0.011\ m^3/kg\text{-}h\ . \qquad (5\text{-}20)$$

Substituting these values into Eq. 5-16 gives the following pathway exposure factors:

$$f_{wa}(child) = 4.6 \times 10^5\ (m^2/s)^{-2/3} \times \left[2.5/D_\ell^{2/3} + RT/\left(D_a^{2/3} H\right)\right]^{-1} (mg/kg\text{-}d)/(mg/L)\ , \qquad (5\text{-}21)$$

$$f_{wa}(adult) = 2.8 \times 10^5\ (m^2/s)^{-2/3} \times \left[2.5/D_\ell^{2/3} + RT/\left(D_a^{2/3} H\right)\right]^{-1} (mg/kg\text{-}d)/(mg/L)\ , \text{ and} \qquad (5\text{-}22)$$

$$F_{wa} = \frac{15}{70} f_{wa}(child) + \frac{55}{70} f_{wa}(adult) \qquad (5\text{-}23)$$

$$= 3.2 \times 10^5\ (m^2/s)^{-2/3} \left[2.5/D_\ell^{2/3} + RT/(D_a^{2/3} H)\right]^{-1} (mg/kg\text{-}d)/mg/L)$$

For organic compounds D_ℓ is on the order of 5×10^{-10} m^2/s and D_a is on the order of 5×10^{-6} m^2/s. If we take the ambient temperature to be 293 K, then equation 5-23 becomes

$$F_{wa} \cong \left[12.4 + \frac{10.6\ RT}{H}\right]^{-1} \text{ (mg/kg-d)/(mg/L)} \qquad (5\text{-}24)$$

when H/RT is large (> 10) this expression gives $F_{wa} \simeq 0.08$. When H/RT is less than approximately 0.05, this expression gives $F_{wa} \simeq 0.004$. In the former case the PEF for water to indoor air F_{wa} is significant relative to the PEF for drinking water ingestion. In the latter case, the water/air PEF, F_{wa}, is small relative to the drinking water PEF F_{ww}.

DERMAL ABSORPTION FROM POTABLE-WATER SUPPLIES

We assume that dermal absorption occurs during bathing and showering. The model used here for dermal absorption from potable water is based on a paper by Brown et al. (1984). In order to make an estimate of the pathway exposure factor for dermal absorption from water, the following simplifying assumptions are made:

- dermal uptake of contaminants occurs mainly by passive diffusion through the stratum corneum,
- resistance to diffusive flux through layers other than the stratum corneum is negligible,
- steady-state diffusive flux is proportional to the concentration difference between water on the skin surface and internal body water,
- children spend approximately the same amount of time bathing, swimming, or showering per week as adults, and
- the amount of time adults spend in showering, bathing, or swimming is equivalent to 80% immersion of the skin surface for a period of 10 min/d in water containing a contaminant at concentration C_w.

This last assumption is intended to represent as much as 20 minutes bathing where, because of evaporative losses, the effective water concentration is on the order 0.5 C_w and to represent a 10-min shower where the contaminant concentration in contact with skin likely remains close to C_w.

The exposure E, in mg/kg-d, from dermal absorption is given by the expression

$$E = J_S T\ f_S\ SA/BW \qquad (5\text{-}25)$$

where

J_S = steady-state flux across the stratum corneum, mg/m^2-h;
T = duration of exposure, h/d;
f_S = fraction of the skin surface immersed in contaminated water, unitless;
SA = surface area of the skin, m^2; and
BW = body weight, kg.

Assuming that chemical transport across the stratum corneum follows Fick's law, the flux, J_S, across the skin is given by

$$J_S = K_p\ \Delta C_{sk} \qquad (5\text{-}26)$$

where

K_p = permeability constant across the stratum corneum, L/m^2-h, and
ΔC_{sk} = concentration difference of the contaminant across the tissue layer, mg/L.

Brown et al. (1984) have determined that K_p is on the order of 10 L/m^2-h for volatile compounds. We assume this number is a first-order approximation for the soluble phase of other water-borne contaminants as well. Furthermore, for dilute solutions we assume that ΔC_{sk} is approximately equal to the chemical concentration in water on the skin surface, C_w. Making the appropriate substitutions in Eq. 5-25 gives

$$E = 10\ L/m^2\text{-h} \times 0.17\ h/d \times 0.80 \times (SA/BW) \times C_w \qquad (5\text{-}27)$$

Substituting values of SA and BW for adults and children as listed in Table 2-2 provides expressions for estimating the two age-specific pathway exposure factors,

$$f_{wd}(child) = E/C_w = 1.36 \frac{L}{m^2\text{-}d} \times \frac{0.95\ m^2}{27\ kg} = 0.048\ (mg/kg\text{-}d)/(mg/L) \quad (5\text{-}28)$$

and

$$f_{wd}(adult) = E/C_w = 1.36 \frac{L}{m^2\text{-}d} \times \frac{1.7\ m^2}{66\ kg} = 0.035\ (mg/kg\text{-}d)/(mg/L) \quad . \quad (5\text{-}29)$$

Finally, the population-equivalent PEF is calculated as

$$F_{wd} = \frac{15}{70} f_{wd}(child) + \frac{55}{70} f_{wd}(adult) = 0.038\ (mg/kg\text{-}d)/(mg/L) \quad . \quad (5\text{-}30)$$

MILK AND MEAT EXPOSURES ATTRIBUTABLE TO CONTAMINATED SURFACE AND GROUND WATER

In this subsection we describe how the concentration of a contaminant in ground water, C_g, or surface water, C_r, can lead to contamination of meat and milk and, thus, lead to human exposures. The concentrations C_w of a contaminant in water supplies results in contaminant concentration in the fresh meat and milk of beef and dairy cattle that use these supplies. These meat and milk concentrations can be related to the concentration C_w using the expressions:

$$C_{mt} = I_{wbc}\ B_t\ C_w \quad (5\text{-}31)$$

$$C_{mk} = I_{wdc}\ B_k\ C_w \quad (5\text{-}32)$$

where

C_{mt} = contaminant concentrations in the fresh meat of beef cattle consuming contaminated water, mg/kg;

C_{mk} = contaminant concentration in the fresh milk of dairy cattle consuming contaminated water, mg/kg;

I_{wbc} = daily intake of water by beef cattle, 44 ± 6.3 L/d (Table 2-7);

I_{wdc} = daily intake of water by dairy cattle, 48 ± 11 L/d (Table 2-7);

B_t = biotransfer factor (see Appendix A) from cattle intake to meat concentration, (mg/kg)/(mg/d); and

B_k = biotransfer factor (see Appendix A) from cattle intake to milk concentration, (mg/kg)/)mg/d).

Using Eqs. 5-31 and 5-32, we can obtain the following expressions for age specific PEFs:

$$f_{wt}\ (child) = (I_t/BW)\ I_{wbc}\ B_t = 0.19\ B_t\ (mg/kg\text{-}d)/(mg/L) \quad (5\text{-}33)$$

$$f_{wt}\ (adult) = (I_t/BW)\ I_{wbc}\ B_t = 0.12\ B_t\ (mg/kg\text{-}d)/(mg/L) \quad (5\text{-}34)$$

$$f_{wk}\ (child) = (I_k/BW)\ I_{wdc}\ B_k = 0.86\ B_k\ (mg/kg\text{-}d)/(mg/L) \quad (5\text{-}36)$$

$$f_{wk}\ (adult) = (I_k/BW)\ I_{wdc}\ B_k = 0.19\ B_k\ (mg/kg\text{-}d)/(mg/L) \quad (5\text{-}36)$$

where

(I_t/BW) = human intake of meat per unit body weight, for children 0.0044 and for adults 0.0028 kg (fresh mass)/kg-d (Table 2-6) and

(I_k/BW) = human intake of dairy products per unit body weight, for children 0.018 and for adults 0.0040 kg (fresh mass)/kg-d (Table 2-6).

When the age-specific PEFs are combined into population equivalent (or lifetime average) PEFs using the appropriate weighting factors, 15/70 for the child PEF and 55/70 for adult PEF, the following expressions result:

$$F_{wt} = 0.14\ B_t \quad (5\text{-}37)$$

$$F_{wk} = 0.33\ B_k \quad (5\text{-}38)$$

6. SUMMARY, DISCUSSION, AND AN EXAMPLE CALCULATION

This report presents methods for integrating multiple exposure routes from multiple environmental media -- namely air, soil, and water -- into a matrix of factors that relate concentrations to human exposure. Each factor in this matrix is referred to as a pathway exposure factor, PEF. The PEF converts a concentration in mg/m^3 in air, mg/L in water, or mg/kg in soil into an equivalent lifetime exposure in mg/kg-d. The previous sections provided step-by-step derivations of the PEFs for air, soil, and water pathways. This section presents a summary of the overall results. The summary is followed by an example that illustrates the application of the PEF approach to three environmental contaminants--arsenic, benzene, and TNT. The section concludes with a discussion of the limitations and implications of using PEFs for assessing human exposure. This discussion focuses on the uncertainties associated with this approach and methods for assessing these uncertainties--methods that are beyond the scope of this report, but are certainly a fertile area for subsequent research efforts.

SUMMARY

The derivation of PEFs may be considered a process consisting of four components. The first of these components involves the organization of environmental concentration data, definition of terms, and review of human and animal physiologic data relevant to integrated exposure assessments. This task is taken up in Section 2. The next three components involve the identification and quantification of exposures attributable to, respectively, air, soil, and water. These three tasks are taken up in Sections 3, 4, and 5.

Section 2 provided the foundation for the models developed in later sections. This section presents an exposure model that considers multiple media and pathways and requires five input contaminant concentrations--concentrations in the (1) gas and (2) particle phases of outdoor air, (3) concentrations in surface soil, (4) concentrations in ground water, and (5) concentrations in surface water. We then identify the units that are assumed in the model for each of these concentrations. Also included with regard to concentrations is a discussion of appropriate measured values,

multimedia simulation models, and methods for estimating dilution factors for atmospheric and ground-water contaminants. Also in Section 2, we defined the terms "exposure," "dose," and "risk" to make clear how they would be used in this report. We provided a review and compilation of human anatomical and dietary parameters needed for exposure estimates. Finally, we presented data on cattle that are relevant for estimating meat and dairy product exposures. The human anatomical data are presented as arithmetic means with corresponding standard deviations. The variance in human anatomical data is combined with variability in uptake and diet parameters in such a way that inhalation, ingestion, and dermal contact could be expressed per unit body weight of adults and children and include estimates of means and standard deviations.

Section 3 described procedures for estimating inhalation and ingestion exposures attributable to contaminants in the gaseous and particle phases of ambient outdoor air. PEFs were developed that relate human exposure through inhalation and ingestion of fruits, vegetables, grains, milk, and meat to atmospheric contamination.

Section 4 described methods for estimating inhalation, ingestion, and dermal absorption exposures attributable to contaminants in the soil surface layer. PEFs were developed to relate soil contamination to indoor inhalation exposures; fruit, vegetable, and grain exposures; and milk exposures that result from plant and soil ingestion by cattle; soil ingestion exposure; and dermal absorption exposure from soil on the skin.

Section 5 was devoted to exposure pathways attributable to contaminated surface and ground water. In that section we developed a PEF that relates fish ingestion exposures to contaminated surface water and PEFs that relate drinking water, milk, and meat ingestion exposures; indoor inhalation exposures; and dermal absorption exposures to contaminated potable-water supplies, which are a mix of ground and surface water.

Table 6-1 provides a matrix that summarizes the values and expressions for the PEFs developed in this report. The listings in this table represent population average or lifetime equivalent PEFs that combine PEFs for adults and children into a single term. The component adult and child PEFs are derived and quantified for each pathway in Sections 3 through 5. Although this report provides data sufficient for estimating the uncertainty associated with each PEF, the task of propagating these uncertainties through the analysis and into the PEF terms is not taken up in this report.

Table 6-1. Summary matrix of values and expressions for the reference population PEFs derived in this report.

	Environmental Concentrations				
	Air (gases) C_a	Air (particles) C_p	Soil C_s	Potable water[a] C_w	Surface water C_r
Pathways	PEF Units = m^3/kg-d	m^3/kg-d	kg/kg-d	L/kg-d	L/kg-d
Inhalation	$F_{aa} = 3.3 \quad 10^{-1}$	$F_{pa} = 3.1 \times 10^{-1}$	$F_{sa} = 9.0 \times 10^{-9}$	$F_{wa} = 3.2 \times 10^{5} \times \left[\frac{2.5}{D_e^{2/3}} + \left(\frac{RT}{H} \times \frac{1}{D_a^{2/3}}\right)\right]^{-1}$	
Ingestion:					
Water				$F_{ww} = 3.4 \times 10^{-2}$	
Fruits					
Vegetables[b]	$F_{av} = 2.5 \times 10^{-6} \times (RT/H) \times (0.9 + 0.1\ K_{ow})$	$F_{pv} = 14$	$F_{sv} = 1.1 \times 10^{-3} \times K_{sp}$		
Grains[b]	$F_{ag} = 3.9 \times 10^{-6} \times (RT/H) \times (0.9 + 0.1\ K_{ow})$	$F_{pg} = 22$	$F_{sg} = 7.9 \times 10^{-4} \times K_{sp}$		
Milk[b]	$F_{ak} = [0.85 + 1.2 \times 10^{-3} \times (RT/H) \times (0.9 + 0.1\ K_{ow})]B_k$	$F_{pk} = 6600 \times B_k$	$F_{sk} = [2.8 \times 10^{-3} + (1.2 \times 10^{-1} \times K_{sp})]B_k$	$F_{wk} = 3.3 \times 10^{-1} \times B_k$	
Meat[b]	$F_{at} = [0.38 + 3.8 \times 10^{-4} (RT/H)] \times (0.9 + 0.1\ K_{ow})]B_t$	$F_{pt} = 2100 \times B_t$	$F_{st} = [1.3 \times 10^{-3} + (3.8 \times 10^{-2} \times K_{sp})]B_t$	$F_{wt} = 1.4 \times 10^{-1} \times B_t$	
Fish			$F_{ss} = 1.5 \times 10^{-6}$		$F_{rf} = 3.2 \times 10^{-4} \times BCF$
Soil				$F_{wd} = 3.8 \times 10^{-2}$	
Dermal absorption			$F_{sd} = 2.6 \times 10^{-6}$		

[a] Potable water concentrations, C_w, are the average of the surface, C_r, and ground water, C_g, concentrations appearing in Table 6-3.
[b] R = 62.4 Torr-L/mol-K; T = 293K.

AN EXAMPLE CALCULATION

This subsection presents a sample calculation that illustrates the use of PEFs for estimating human exposure to three toxic but chemically different species--arsenic, benzene, and TNT. Arsenic and benzene are known human carcinogens; military-grade TNT (containing TNT isomers and isomers of dinitrotoluene as impurities) has caused malignant tumors in mice and rats in chronic toxicity studies (see Layton et al., 1987). Benzene is a volatile organic chemical that degrades in the atmosphere. When released to the environment it tends to move from soil and water into the atmosphere. TNT is much less volatile and tends to accumulate more in soil and water than in air. It degrades to other aromatic compounds in soil and surface water. Arsenic is an element and thus a stable species. Its movement in the environment is governed by its solubility and its attachment to mobile particles. We do not intend our exposure calculations for these contaminants to provide definitive estimates of potential human exposures, but instead to demonstrate the use of the formulae in Table 6-1 for making preliminary estimates of the significance of a number of potential pathways. In the paragraphs below, we will calculate exposures by environmental media (air, soil, water) for each contaminant. After this we will compare the relative contributions to total exposure for each species by pathway (inhalation, ingestion, dermal absorption).

Table 6-2 lists the physicochemical properties of the three contaminants used in this exercise. Table 6-3 lists environmental concentrations in air, soil, and water used for the sample calculations. These values were obtained using the GEOTOX program with steady-state inputs of the contaminants to the soil compartment. The resulting concentrations correspond to the equilibrium distribution of each contaminant among the environmental system modelled in GEOTOX. The landscape data used for this calculation were compiled by Layton et al. (1986) to represent the northeastern and central regions of the United States. The results of the calculation were scaled so that the soil concentration for each contaminant equals 1 ppm (mg/kg). The results reveal that, in terms of concentration, arsenic tends to concentrate in the soil compartment; benzene tends to concentrate in the atmosphere and to a lesser extent in soil and water (it should be noted that 1 mg/m^3 in air is approximately equal to the concentration by mass of 1 mg/kg in soil); and TNT

Table 6-2. Physicochemical properties of the candidate species.

Property	Units	Symbol	Values[a] Arsenic	Benzene	TNT
Molecular weight	g	MW	74.9	78.1	227
Henry's law constant	torr-L/mol	H	~0	4.1×10^{3}	2.0×10^{-3}
Octanol/water partition factor	unitless	K_{ow}	--	135	39.8
Organic carbon partition factor	unitless	K_{oc}	--	76	534
Soil/water sorption coefficient	L/kg	K_d	1300	--	--
Diffusion coefficient (air)	m^2/s	D_a	$\sim 10^{-6}$	5.0×10^{-6}	5.9×10^{-6}
Diffusion coefficient (water)	m^2/s	D_ℓ	$\sim 10^{-10}$	5.0×10^{-10}	5.8×10^{-10}
Soil/plant partition coefficient (dry mass)	unitless	K_{sp}	0.11	4.34	6.3
Bioconcentration factor in fish	L/kg	BCF	75	75	10
Meat/diet biotransfer factor in cattle	d/kg	B_t	6.2×10^{-5}[b]	1.3×10^{-4}[c]	7.2×10^{-5}[c]
Milk/diet biotransfer factor in cattle	d/L	B_k	6.2×10^{-5}[d]	1.2×10^{-5}[e]	6.5×10^{-6}[e]

[a] Unless otherwise noted these values for arsenic and benzene are derived from Layton et al., (1986), while the values for TNT are from Layton et al. (1987).

[b] Assumed that B_t for arsenic is equivalent to B_k for arsenic (see footnote "[d]").

[c] Calculated using Equation A-7 (see Appendix A).

[d] Taken from Table A-1 (see Appendix A).

[e] Calculated using Equation A-8 (see Appendix A).

Table 6-3. Steady-state environmental concentrations used in the sample calculations. Concentrations are predicted using the GEOTOX model with parameter inputs from Table 6-2 (see text for details).

Description	Units	Symbol	Values		
			Arsenic	Benzene	TNT
Concentration of contaminant in air	mg/m^3	C_a	~0	23	2.5×10^{-8}
Concentration of contaminant in air and attached to dust particles	mg/m^3	C_p	5.2×10^{-8}	4.2×10^{-8}	5.0×10^{-8}
Concentration of contaminant in soil	mg/kg	C_s	1.0	1.0	1.0
Concentration of contaminant in ground water	mg/L	C_g	1.0×10^{-3}	0.62	0.10
Concentration of contaminant in surface water	mg/L	C_r	1.8×10^{-3}	0.59	0.0043
Concentration of contaminant in potable water[a]	mg/L	C_w	1.4×10^{-3}	0.61	0.052

[a] Concentrations in potable water, C_w, are taken to be the average of the surface, C_r, and ground water, C_g, concentrations.

tends to concentrate in soil and ground water. Using the formulae in Table 6-1 and the data in Tables 6-2 and 6-3, we estimate exposures by environmental medium and exposure pathway.

Exposures Associated with Contaminants in Air

Exposures attributable to contaminants in air are estimated using the expressions in the first two columns of Table 6-1

$$E^a(C_a, C_p) = e^a_h(C_a, C_p) + e^a_g(C_a, C_p) \qquad (6\text{-}1)$$

where

$E^a(C_a, C_p)$ = total exposure attributable to contaminant concentrations C_a and C_p in air, mg/kg-d;

$e_h^a(C_a, C_p)$ = inhalation exposure attributable to contaminant concentrations C_a and C_p in air, mg/kg-d; and

$e_g^a(C_a, C_p)$ = ingestion exposure attributable to contaminant concentrations C_a and C_p in air, mg/kg-d.

The inhalation exposures are the sum of contributions from gases and particles

$$e_h^a(C_a, C_p) = F_{aa} C_a + F_{pa} C_p \quad . \tag{6-2}$$

Making the appropriate substitutions from Tables 6-1 and 6-2 for each of the contaminants gives

$$e_h^a(C_a, C_p) = 0.39 \times 0.0 + 0.31 \times 5.2 \times 10^{-8}$$
$$= 1.6 \times 10^{-8} \text{ mg/kg-d (arsenic)} \tag{6-3}$$

$$e_h^a(C_a, C_p) = 0.39 \times 23 + 0.31 \times 4.2 \times 10^{-8}$$
$$= 9.0 \text{ mg/kg-d (benzene)} \tag{6-4}$$

$$e_h^a(C_a, C_p) = 0.39 \times 2.5 \times 10^{-8} + 0.31 \times 5.0 \times 10^{-8}$$
$$= 2.5 \times 10^{-8} \text{ mg/kg-d (TNT)} \tag{6-5}$$

The ingestion exposures are constructed from Table 6-1 as

$$e_g^a(C_a, C_p) = (F_{av} + F_{ag} + F_{ak} + F_{at})C_a + (F_{pv} + F_{pg} + F_{pk} + F_{pt})C_p \tag{6-6}$$

Making the appropriate substitutions gives

$$e_g^a(C_a, C_p) = [14 + 22 + (6600\ B_k) + (2100\ B_t)]C_p$$
$$= [14 + 22 + (6600 \times 6.2 \times 10^{-5}) + (2100 \times 6.2 \times 10^{-5})] \times 5.2 \times 10^{-8}$$
$$= 1.9 \times 10^{-6} \text{ mg/kg-d (arsenic)} \tag{6-7}$$

$$e_g^a(C_a, C_g) = \Big\{2.5 \times 10^{-6}\ (RT/H)(0.9 + 0.1\ K_{ow}) + 3.9 \times 10^{-6}\ (RT/H)$$
$$(0.9 + 0.1\ K_{ow}) + [8.5 \times 10^{-1} + 1.2 \times 10^{-3}\ (RT/H)$$
$$(0.9 + 0.1\ K_{ow})]\ B_k + [3.8 \times 10^{-1} + 3.8 \times 10^{-4})(RT/H)$$
$$(0.9 + 0.1\ K_{ow})]\ B_t\Big\}\ C_a + [14 + 22 + (6600\ B_k) +$$
$$(2100\ B_t)]\ C_p =$$
$$\Big\{2.5 \times 10^{-6}\ (4.4)(14) + 3.9 \times 10^{-6}\ (4.4)(14) +$$
$$[8.5 \times 10^{-1} + 1.2 \times 10^{-3}\ (4.4)(14)]\ 1.2 \times 10^{-5} +$$
$$[3.8 \times 10^{-1} + 3.8 \times 10^{-4}\ (4.4)\ (14)]\ 1.3 \times 10^{-4}\Big\} \times 23 +$$
$$[14 + 22 + 6600 \times 1.2 \times 10^{-5} + 2100 \times 1.3 \times 10^{-4}] \times$$
$$4.2 \times 10^{-8} =$$
$$[1.5 \times 10^{-4} + 2.4 \times 10^{-4} + 1.1 \times 10^{-5} + 5.2 \times 10^{-5}] \times 23 +$$
$$36 \times 4.2 \times 10^{-8} =$$
$$1.0 \times 10^{-2}\ \text{mg/kg-d (benzene)} \qquad (6\text{-}8)$$

$$e_g^a(C_a, C_p) = \Big\{2.5 \times 10^{-6}\ (9.1 \times 10^6)(4.9) + 3.9 \times 10^{-6}\ (9.1 \times 10^6)$$
$$(4.9) + [8.5 \times 10^{-1} + (1.2 \times 10^{-3})(9.1 \times 10^6)\ (4.9)] \times$$
$$6.5 \times 10^{-6} + [3.8 \times 10^{-1} + 3.8 \times 10^{-4}\ (9.1 \times 10^6)$$
$$(4.9)]\ 7.2 \times 10^{-5}\Big\} \times 2.5 \times 10^{-8} + [14 + 22 + 6600 \times$$
$$6.5 \times 10^{-6} + 2100 \times 7.2 \times 10^{-5}] \times 5.0 \times 10^{-8} =$$
$$(110 + 170 + 0.35 + 1.2) \times 2.5 \times 10^{-8} +$$
$$36 \times 5.0 \times 10^{-8} =$$
$$8.8 \times 10^{-6}\ \text{mg/kg-d (TNT)} \qquad (6\text{-}9)$$

In reviewing these calculations, the reader should note that the inhalation exposure to arsenic depends only on the particle-phase concentration, inhalation exposure to benzene depends only on the gas-phase component of atmospheric concentration and inhalation exposure to TNT depends on both particles and gases. The ingestion exposure for arsenic is strongly dependent

on the deposition of particles to vegetation; for benzene, on deposition of gases to vegetation; and for TNT, on deposition of both particles and gases onto vegetation.

The total exposure attributable to atmospheric contaminants can now be calculated

$$E^a(C_a, C_p) = e_h^a(C_a, C_p) + e_g^a(C_a, C_p) \quad (6\text{-}10)$$

$$E^a(C_a, C_p) = (1.6 \times 10^{-8}) + (1.9 \times 10^{-6})$$
$$= 1.9 \times 10^{-6} \text{ mg/kg-d (arsenic)}; \quad (6\text{-}11)$$

$$E^a(C_a, C_p) = 9.0 + (1 \times 10^{-2}) = 9.0 \text{ mg/kg-d (benzene)}; \text{ and} \quad (6\text{-}12)$$

$$E^a(C_a, C_p) = (2.5 \times 10^{-8}) + (8.8 \times 10^{-6}) = 8.8 \times 10^{-6} \text{ mg/kg-d (TNT)} \quad (6\text{-}13)$$

These results indicate that, for arsenic and TNT, ingestion is the dominant pathway for human exposure to atmospheric contaminants. Whereas, for benzene inhalation is the dominant exposure pathway to atmospheric contaminants.

Exposures Associated with Contaminated Soil

As shown in Section 4, exposures attributable to contaminated soil can be divided into inhalation, ingestion, and dermal absorption exposures:

$$E^s(C_s) = e_h^s(C_s) + e_g^s(C_s) + e_d^s(C_s) \quad (6\text{-}14)$$

where

$E^s(C_s)$ = total exposure attributable to the contaminant concentration C_s in soil, mg/kg-d;

$e_h^s(C_s)$ = inhalation exposure attributable to the contaminant concentration C_s in soil, mg/kg-d;

$e_g^s(C_s)$ = ingestion exposure attributable to the contaminant concentration C_s in soil, mg/kg-d; and

$e_d^s(C_s)$ = dermal absorption exposure attributable to the contaminant concentration C_s in soil, mg/kg-d.

Based on the derivations in Section 4 and the summary of these results in Table 6-1, the inhalation exposure is given by

$$e_h^s(C_s) = F_{sa} C_s \quad . \tag{6-15}$$

Making the appropriate substitutions from Tables 6-1 and 6-3 gives

$$e_h^s(C_s) = 9.0 \times 10^{-9} \times 1.0 = 9.0 \times 10^{-9} \tag{6-16}$$

for arsenic, benzene, and TNT.

The ingestion exposures are constructed from Table 6-1 as

$$e_g^s(C_s) = (F_{sv} + F_{sg} + F_{sk} + F_{st} + F_{ss}) C_s \tag{6-17}$$

which can be expanded to

$$e_g^s(C_s) = [1.1 \times 10^{-3} K_{sp} + 7.9 \times 10^{-4} K_{sp} + (0.0028 + 0.12 K_{sp}) B_k + (0.0013 + 0.038 K_{sp}) B_t + 1.5 \times 10^{-6}] C_s \tag{6-18}$$

Making the appropriate substitutions from Tables 6-2 and 6-3 gives

$$\begin{aligned} e_g^s(C_s) &= [(1.1 \times 10^{-3} + 7.9 \times 10^{-4}) \times 0.11 + (0.0028 + 0.12 \times 0.11) \times \\ &\quad 6.2 \times 10^{-5} + (0.0013 + 0.038 \times 0.11) \times 6.2 \times 10^{-5} + \\ &\quad 1.5 \times 10^{-6}] \times 1.0 \\ &= 2.1 \times 10^{-4} \text{ mg/kg-d for arsenic,} \end{aligned} \tag{6-19}$$

$$\begin{aligned} e_g^s(C_s) &= [(1.1 \times 10^{-3} + 7.9 \times 10^{-4}) \times 4.34 + \\ &\quad (0.0028 + 0.12 \times 4.34) \times 1.2 \times 10^{-5} + \\ &\quad (0.0013 + 0.038 \times 4.34) \times 1.3 \times 10^{-4} + 1.5 \times 10^{-6}] \times 1.0 \\ &= 8.2 \times 10^{-3} \text{ mg/kg-d for benzene, and} \end{aligned} \tag{6-20}$$

$$\begin{aligned} e_g^s(C_s) &= [(1.1 \times 10^{-3} + 7.9 \times 10^{-4}) \times 6.3 + \\ &\quad (0.0028 + 0.12 \times 6.3) \times 6.5 \times 10^{-6} + \\ &\quad (0.0013 + 0.038 \times 6.3) \times 7.2 \times 10^{-5} + 1.5 \times 10^{-6}] \times 1.0 \\ &= 1.2 \times 10^{-2} \text{ mg/kg-d for TNT.} \end{aligned} \tag{6-21}$$

The dermal absorption exposure associated with contaminated soil is constructed from Table 6-1 as

$$e_d^s(C_s) = F_{sd} C_s = 2.6 \times 10^{-6} C_s \tag{6-22}$$

Because C_s = 1.0 mg/kg for all three species--arsenic, benzene, and TNT; the exposure for all three is equal to 2.6×10^{-6} mg/kg-d.

Exposures Associated with Contaminants in Water

Exposures associated with contaminants in ground and surface waters and the resulting potable water supplies are discussed in Section 5 and include inhalation, ingestion, and dermal absorption exposures:

$$E^w(C_w, C_r) = e_h^w(C_w) + e_g^w(C_w, C_r) + e_d^w(C_w) \quad (6\text{-}23)$$

where

$E^w(C_w, C_r)$ = total exposure attributable to the contaminant concentration C_w in potable-water and C_r in surface waters, mg/kg-d;

$e_h^w(C_w)$ = inhalation exposure attributable to the contaminant concentration C_w in potable-water supplies, mg/kg-d;

$e_g^w(C_w, C_r)$ = ingestion exposure attributable to the contaminant concentration C_w in potable-water supplies and C_r in surface waters, mg/kg-d; and

$e_d^w(C_w)$ = dermal absorption exposure attributable to the contaminant concentration C_w in potable-water supplies, mg/kg-d.

Based on the discussion in Section 5 and the summary of the results of this work in Table 6-1, the inhalation exposure for the water pathway can be estimated using the expression:

$$e_h^w(C_w) = F_{wa} C_w = 3.2 \times 10^5 \times \left[2.5/D_\ell^{2/3} + RT/(D_a^{2/3} H)\right]^{-1} C_w. \quad (6\text{-}24)$$

The gas constant R is 62.4 mol-L/torr-K and we assume a temperature of 293 K. This information, combined with the appropriate substitutions from Tables 6-2 and 6-3, gives the following expressions:

$$e_h^w (C_w) = 3.2 \times 10^5 \left[2.5/(10^{-10})^{2/3} + 62.4 \times 293/\left((10^{-6})^{2/3} \times 0\right)\right]^{-1} \times 1.4 \times 10^{-3} \quad (6\text{-}25)$$

~ 0 for arsenic.

$$e_h^w (C_w) = 3.2 \times 10^5 \left[2.5/(5 \times 10^{-10})^{2/3} + 62.4 \times 293/((5 \times 10^{-6})^{2/3} \times 4.1 \times 10^3)\right]^{-1} \times 0.61$$

$$= 1.95 \times 10^5/(4.0 \times 10^6 + 1.5 \times 10^4)$$
$$= 4.9 \times 10^{-2} \text{ mg/kg-d for benzene, and} \quad (6\text{-}26)$$

$$e_h^w (C_w) = 3.2 \times 10^5 \left[2.5/(5.8 \times 10^{-10})^{2/3} + 62.4 \times 293/((5.9 \times 10^{-6})^{2/3} \times 2.0 \times 10^{-3})\right]^{-1} \times 0.052$$

$$= 1.7 \times 10^4/(3.6 \times 10^6 + 2.8 \times 10^{10})$$

$$= 6.0 \times 10^{-7} \text{ mg/kg-d for TNT.} \quad (6\text{-}27)$$

It should be noted that for benzene the inhalation exposure is determined by the liquid-side mass transfer (the first term in the brackets Eq. 6-26) whereas for TNT the inhalation exposure is determined by the gas-side mass transfer (the second term in the brackets in Eq. 6-27). However, the overall TNT inhalation exposure is five orders of magnitude lower than that for benzene and not a significant contribution when compared to other exposure routes (ingested and dermal) associated with potable water.

The ingestion exposures are constructed from Table 6-1 to form the expression,

$$e_g^w (C_w, C_r) = (F_{ww} + F_{wk} + F_{wt})\, C_w + F_{rf}\, C_r \qquad (6\text{-}28)$$

Based on the last two columns of Table 6-1, this expression becomes

$$e_g^w (C_w, C_r) = (0.034 + 0.33\, B_k + 0.14\, B_t)\, C_w + 3.2 \times 10^{-4}\, BCF\, C_r \qquad (6\text{-}29)$$

Making the appropriate substitutions from Tables 6-2 and 6-3 allows quantitative estimates of these exposures,

$$e_g^w (C_w, C_r) = (0.034 + 0.33 \times 6.2 \times 10^{-5} + 0.14 \times 6.2 \times 10^{-5}) \times 1.4 \times 10^{-3} + 3.2 \times 10^{-4} \times 75 \times 1.8 \times 10^{-3}$$
$$= 9.1 \times 10^{-5} \text{ mg/kg-d for } \underline{\text{arsenic}}, \qquad (6\text{-}30)$$

$$e_g^w (C_w, C_r) = (0.034 + 0.33 \times 1.2 \times 10^{-5} + 0.14 \times 1.3 \times 10^{-4}) \times 0.61 + 3.2 \times 10^{-4} \times 75 \times 0.59$$
$$= 3.5 \times 10^{-2} \text{ mg/kg-d for } \underline{\text{benzene}}, \text{ and} \qquad (6\text{-}31)$$

$$e_g^w (C_w, C_r) = (0.034 + 0.33 \times 6.5 \times 10^{-6} + 0.14 \times 7.2 \times 10^{-5}) \times 0.052 + 3.2 \times 10^{-4} \times 10 \times 0.0043$$
$$= 1.8 \times 10^{-3} \text{ mg/kg-d for } \underline{\text{TNT}}. \qquad (6\text{-}32)$$

The dermal absorption exposure associated with contaminated potable water is estimated using the expression

$$e_d^w (C_w) = F_{wd} C_w = 0.038 C_w \quad (6\text{-}33)$$

Making the appropriate substitutions gives

$$e_d^w = 0.038 \times 1.4 \times 10^{-3} = 5.3 \times 10^{-5} \text{ mg/kg-d} \quad \text{for arsenic,} \quad (6\text{-}34)$$

$$e_d^w = 0.038 \times 0.61 = 2.3 \times 10^{-2} \text{ mg/kg-d} \quad \text{for benzene, and} \quad (6\text{-}35)$$

$$e_d^w = 0.038 \times 0.052 = 2.0 \times 10^{-3} \text{ mg/kg-d} \quad \text{for TNT.} \quad (6\text{-}36)$$

Summary of the Example Calculation

The PEFs used for arsenic, benzene and TNT in the example calculation are summarized in Tables 6-4, 6-5, and 6-6. The results of the sample calculation of exposure for arsenic, benzene, and TNT are summarized respectively in Tables 6-7, 6-8, and 6-9.

Examination of the results in Table 6-7 reveals that, for arsenic, ingestion is the dominant route of exposure followed by dermal absorption. The ingestion exposure is contributed by soil-based and water-based pathways, specifically the ingestion of fruits, vegetables, and grains: the intake of drinking water and the ingestion of fish.

The results in Table 6-8 indicate that, for benzene, inhalation of ambient air is the dominant exposure followed by inhalation of benzene transfered from tap water to indoor air. It is of interest that, among the water-based pathways, indoor inhalation and dermal absorption are as important as ingestion. Among the soil-based pathways, ingestion of fruits, vegetables, and grains dominates over all other exposure routes. It is also of interest that the ingestion exposure to benzene is more than an order of magnitude larger than that for arsenic when the soil concentration for both compounds is 1 ppm. This observation indicates the importance of physicochemical properties for defining the availability of chemical species for human exposure.

Table 6-4. Summary of pathway exposure factors (PEFs) and estimated exposures for gases and particles in air.

PEF	Arsenic	Benzene	TNT
C_a	0.0	2.3×10^{1}	2.5×10^{-8}
C_p	5.2×10^{-8}	4.2×10^{-8}	5.0×10^{-3}
F_{aa}	3.9×10^{-1}	3.9×10^{-1}	3.9×10^{-1}
$F_{aa} \times C_a$	0.0	9.0×10^{0}	9.8×10^{-9}
F_{pa}	3.1×10^{-1}	3.1×10^{-1}	3.1×10^{-1}
$F_{pa} \times C_p$	1.6×10^{-8}	1.3×10^{-8}	1.6×10^{-8}
$e_h^a(C_a, C_p) = F_{aa}C_a + F_{pa}C_p$	1.6×10^{-8}	9.0×10^{0}	2.5×10^{-8}
F_{av}	---	1.5×10^{-4}	1.1×10^{2}
F_{ag}	---	2.4×10^{-4}	1.7×10^{2}
F_{ak}	---	1.1×10^{-5}	3.5×10^{-1}
F_{at}	---	5.2×10^{-5}	1.2×10^{0}
F_{pv}	1.4×10^{1}	1.4×10^{1}	1.4×10^{1}
F_{pg}	2.2×10^{1}	2.2×10^{1}	2.2×10^{1}
F_{pk}	4.1×10^{-1}	7.9×10^{-2}	4.3×10^{-2}
F_{pt}	1.3×10^{-1}	2.7×10^{-1}	1.5×10^{-1}
$e_h^a(C_a, C_p) = (F_{av} + F_{ag} + F_{ak} + F_{at}) C_a + (F_{pv} + F_{pg} + F_{pk} + F_{pt}) C_p$	1.9×10^{-6}	1.0×10^{-2}	8.8×10^{-6}

Table 6-9 reveals that, for TNT, overall exposure is mainly attributable to ingestion and dermal absorption, with inhalation exposure expected to be several orders of magnitude lower. The dermal absorption exposure is dominated by the water-based absorption route. Important contributions to ingestion come from both soil- and to a lesser extent water-based pathways. The soil-based ingestion pathways are dominated by the intake of fruits, vegetables and grains. The water-based pathway is almost completely attributable to the intake of potable water.

Table-6-5. Summary of pathway exposure factors (PEFs) and estimated exposures for soil.

PEF	Arsenic	Benzene	TNT
C_s	1.0	1.0	1.0
F_{sa}	9.0×10^{-9}	9.0×10^{-9}	9.0×10^{-9}
$e_h^s(C_s) = F_{sa}C_s$	9.0×10^{-9}	9.0×10^{-9}	9.0×10^{-9}
F_{sv}	1.2×10^{-4}	4.8×10^{-3}	6.9×10^{-3}
F_{sg}	8.7×10^{-5}	3.4×10^{-3}	5.0×10^{-3}
F_{sk}	9.9×10^{-7}	6.3×10^{-6}	4.9×10^{-6}
F_{st}	3.4×10^{-7}	2.2×10^{-5}	1.7×10^{-5}
F_{ss}	1.5×10^{-6}	1.5×10^{-6}	1.5×10^{-6}
$e_g^s(C_s) = (F_{sv} + F_{sg} + F_{sk} + F_{st} + F_{ss})\, C_s$	2.1×10^{-4}	8.2×10^{-3}	1.2×10^{-2}
F_{sd}	2.6×10^{-6}	2.6×10^{-6}	2.6×10^{-6}
$e_d^s(C_s) = F_{sd}C_s$	2.6×10^{-6}	2.6×10^{-6}	2.6×10^{-6}

DISCUSSION AND CONCLUSIONS

The goals of this report are to outline a procedure for estimating human exposure from multiple pathways, provide preliminary methods for estimating exposure through each pathway, and illustrate the use of these methods with some examples. These are rather ambitious goals and the scope of the current report makes it impossible to address all of the problems associated with the process of performing an integrated multimedia-exposure assessment. Nonetheless, we believe the report is complete in the sense that it has listed and addressed all of the potential pathways of human exposure for toxic chemicals found in the environment.

Table 6-6. Summary of pathway exposure factors (PEFs) and estimated exposures for surface water (C_r) and tap water (C_w).

PEF	Arsenic	Benzene	TNT
C_w	1.4×10^{-3}	6.1×10^{-1}	5.2×10^{-2}
F_{wa}	1.8×10^{-9}	8.0×10^{-2}	1.1×10^{-5}
$e_h^w(C_w) = F_{wa}C_w$	~0	4.9×10^{-2}	6.0×10^{-7}
F_{ww}	3.4×10^{-2}	3.4×10^{-2}	3.4×10^{-2}
F_{wk}	2.0×10^{-5}	4.0×10^{-6}	2.1×10^{-6}
F_{wt}	8.7×10^{-6}	1.8×10^{-5}	1.0×10^{-5}
F_{rf}	2.4×10^{-2}	2.4×10^{-2}	3.2×10^{-3}
C_r	1.8×10^{-3}	5.9×10^{-1}	4.3×10^{-3}
$e_g^w = (F_{ww} + F_{wk} + F_{wt})C_w + F_{rf}C_r$	9.1×10^{-5}	3.5×10^{-2}	1.8×10^{-3}
F_{wd}	3.8×10^{-2}	3.8×10^{-2}	3.8×10^{-2}
$e_d^w = F_{wd}C_w$	5.3×10^{-5}	2.3×10^{-2}	2.0×10^{-3}

One of the fundamental assumptions made in this report is that all the pathways are fully available. That is, the individual at risk is assumed to obtain all of his or her air, water, and food from an environment having the specified contaminant concentrations in the air, water, and soil. Except for contaminants that are uniformly released and spread over a large region, this is not likely to be the case. A more realistic approach to assessing human exposures requires that we now go back to the expression for each exposure route and prescribe methods for adjusting these expressions to account for the variability of individual exposure that is attributable to spatial variation in concentration and the time dependence of pathways. One approach to this problem, that is compatible with the PEF approach, is to specify the concentrations in each medium (air, soil, water) as a probability distribution, which characterizes the variation of concentrations as a result of population movement, individual life styles (i.e., food supply, housing, and water supply choices), and the time and spatial character of the source.

Table 6-7. Exposure matrix for arsenic.

Pathway	Exposure by environmental compartment (values in mg/kg-d)				
	Air (gases)	Air (particles)	Soil	Water	Total
Inhalation	--	1.6×10^{-8}	9.0×10^{-9}	0	2.5×10^{-8}
Ingestion					
Water	--	--	--	4.8×10^{-5}	4.8×10^{-5}
Fruits, vegetables	--	7.3×10^{-7}	1.2×10^{-4}	--	1.2×10^{-4}
Grains	--	1.1×10^{-6}	8.7×10^{-5}	--	8.8×10^{-5}
Milk	--	2.1×10^{-8}	9.9×10^{-7}	2.9×10^{-8}	1.0×10^{-6}
Meat	--	6.8×10^{-9}	3.4×10^{-7}	1.2×10^{-8}	3.6×10^{-7}
Fish	--	--	--	4.3×10^{-5}	4.3×10^{-5}
Soil	--	--	1.5×10^{-6}	--	1.5×10^{-6}
Total Ingestion	--	1.9×10^{-6}	2.1×10^{-4}	9.1×10^{-5}	3.0×10^{-4}
Dermal absorption	--	--	2.6×10^{-6}	5.3×10^{-5}	5.6×10^{-5}
Totals	0	1.9×10^{-6}	2.1×10^{-4}	1.4×10^{-4}	3.6×10^{-4}

As we have stated, the goal of this report is to assemble available references to provide as complete a picture of human exposure as is possible for preliminary estimates. Some of the PEFs are based on more certain data and more realistic models than others. Listed below are issues that limit the utility of several of the PEFs described in the report.

- The soil/plant partition coefficient K_{sp} that expresses the partitioning of contaminants between soil and food and pasture crops is not well known for most compounds. Using what is known about

Table 6-8. Exposure matrix for benzene.

Pathway	Exposure by environmental compartment (values in mg/kg-d)				
	Air (gases)	Air (particles)	Soil	Water	Total
Inhalation	9.0	1.3×10^{-8}	9.0×10^{-9}	4.9×10^{-2}	9.0
Ingestion					
Water	--	--	--	2.1×10^{-2}	2.1×10^{-2}
Fruits, vegetables	3.4×10^{-3}	5.9×10^{-7}	4.8×10^{-3}	--	8.2×10^{-3}
Grains	5.5×10^{-3}	9.2×10^{-7}	3.4×10^{-3}	--	8.9×10^{-3}
Milk	2.5×10^{-4}	3.3×10^{-9}	6.3×10^{-6}	2.4×10^{-6}	2.6×10^{-4}
Meat	1.2×10^{-3}	1.1×10^{-8}	2.2×10^{-5}	1.1×10^{-5}	1.2×10^{-3}
Fish	--	--	--	1.4×10^{-2}	1.4×10^{-2}
Soil	--	--	1.5×10^{-6}	--	1.5×10^{-6}
Total Ingestion	1.0×10^{-2}	1.5×10^{-6}	8.2×10^{-3}	3.5×10^{-2}	5.3×10^{-2}
Dermal absorption	--	--	2.6×10^{-6}	2.3×10^{-2}	2.3×10^{-2}
Totals	9.0	1.5×10^{-6}	8.2×10^{-3}	1.1×10^{-1}	9.1

chemicals for which this parameter has been measured provides a way of setting upper and lower limits on K_{sp}, but for many compounds the uncertainty in K_{sp} can be orders of magnitude. This has important implications for any compound for which the ingestion of meat, milk, fruits, vegetables, and grains is likely to be an important pathway.

- The biotransfer factors B_t and B_k, which express contaminant partitioning between cattle diet and meat and milk, can probably only be estimated within about two orders of magnitude for many chemical species. This limitation has important implications for situations where these are potentially important pathways.

Table 6-9. Exposure matrix for TNT.

Pathway	Exposure by environmental compartment (values in mg/kg-d)				
	Air (gases)	Air (particles)	Soil	Water	Total
Inhalation	9.8×10^{-9}	1.6×10^{-8}	9.0×10^{-9}	6.0×10^{-7}	6.3×10^{-7}
Ingestion					
Water	--	--	--	1.8×10^{-3}	1.8×10^{-3}
Fruits, vegetables	2.7×10^{-6}	7.0×10^{-7}	6.9×10^{-3}	--	6.9×10^{-3}
Grains	4.3×10^{-6}	1.1×10^{-6}	5.0×10^{-3}	--	5.0×10^{-3}
Milk	8.7×10^{-9}	2.1×10^{-9}	4.9×10^{-6}	1.1×10^{-7}	5.0×10^{-6}
Meat	3.0×10^{-8}	7.6×10^{-9}	1.7×10^{-5}	5.3×10^{-7}	1.8×10^{-5}
Fish	--	--	--	1.4×10^{-5}	1.4×10^{-5}
Soil	--	--	1.5×10^{-6}	--	1.5×10^{-6}
Total Ingestion	7.0×10^{-6}	1.8×10^{-6}	1.2×10^{-2}	1.8×10^{-3}	1.4×10^{-2}
Dermal absorption	--	--	2.6×10^{-6}	2.0×10^{-3}	2.0×10^{-3}
Totals	7.0×10^{-6}	1.8×10^{-6}	1.2×10^{-2}	3.8×10^{-3}	1.6×10^{-2}

- The dermal absorption of chemicals from bath and shower water is based on limited data defining the permeability of the skin to chemical transport. The estimate for this parameter used here was based on the few measurements presented in the literature for a limited number of volatile organic chemicals. It is likely that the uncertainty associated with this model results in a large uncertainty in the resulting estimate of human exposure. However, because the model in question is conservative, it is likely that improving the resolution of this pathway would result in substantially lower estimates of exposure by this route. This issue gains importance given that two of the chemicals in the example calculation, arsenic and TNT, showed dermal absorption from water to be a major exposure route.

It appears that one of the most important next steps is a systematic evaluation of uncertainties. This report has laid some of the groundwork for this process. In Section 2, we reported human inhalation and ingestion parameters as the arithmetic means of probability distributions and reported the corresponding standard deviations. It remains for someone to develop such distributions for the many other parameters used in the integrated exposure assessment. Once this is done, it will be possible to calculate the uncertainty in each PEF and identify the principal sources of the uncertainties. Using this procedure, one can identify parameters that must be better characterized when making decisions about managing health risk through exposure reductions. It is difficult to make more definitive conclusions about the results of this work until such sensitivity/uncertainty analyses are completed.

There are, however, some conclusions that can be drawn regarding the expressions in Table 6-1 and the results of the example calculation as summarized in tables 6-7 through 6-9. Listed below are some of the more impcrtant conclusions:

- Dermal absorption of chemicals from soil is not likely to be an important exposure route unless all other soil and water pathways are unavailable. As revealed in the example calculations, the dermal absorption of contaminants from soil is expected to be at least two orders of magnitude and perhaps over four orders of magnitude lower than the total soil-based exposure.

- Inhalation of volatile organic chemicals (VOCs) transported from potable-water supplies to indoor air has the potential for being as important an exposure route as the direct ingestion of VOCs from potable-water supplies

- When addressing the intake of chemical species through milk and meat, it is important to consider all potential intake routes for these chemicals by cattle. For someone first addressing this problem, it would seem obvious to assume that the principal source of contaminants for cattle is contaminated pasture. However, the example calculations here indicate that the atmosphere can provide a source for volatile compound like benzene in the milk or meat of

cattle through inhalation of the benzene by cattle. For TNT and arsenic both soil and water provide sources of contaminants expected in the milk and meat supply. In addition, the soil provides a source of contaminants both through soil/plant transfers and through direct ingestion of soil by cattle.

ACKNOWLEDGMENT

Parts of this report were prepared while the author, T.E. McKone, was at Harvard University and supported by Grant CR-812699 to the Interdisciplinary Programs in Health by the U.S. Environmental Protection Agency (U.S. EPA). However, this report does not necessarily represent the views and policies of the U.S. EPA.

APPENDIX A

Calculation of Biotransfer Factors in Fat, Meat, and Milk Derived from Cattle

The purpose of this appendix is to develop methods for estimating biotransfer factors (BTFs) for chemical elements and organic compounds in meat, milk, and (in the case of organics) fat tissue of beef and dairy cattle. The traditional measure of a contaminant's potential to accumulate in an organism is the bioconcentration factor (BCF), which is defined as a contaminant's concentration in an organism or tissue divided by its concentration in water (for aquatic organisms) or in food (for terrestrial organisms). However, the concept of BTF is more useful in exposure assessments in which we are considering exposures to cattle from multiple media such as inhalation, grazing, soil ingestion, and water pathways. In this situation a simple ratio is difficult to apply.

BTFs for meat (B_t), milk (B_k), and cattle fat (B_f) are defined as

$$B_t = \frac{\text{contaminant concentration in meat (mg/kg)}}{\text{daily contaminant intake (mg/d)}} \quad \text{(A-1)}$$

$$B_k = \frac{\text{contaminant concentration in milk (mg/kg)}}{\text{daily contaminant intake (mg/d)}} \quad \text{(A-2)}$$

$$B_f = \frac{\text{contaminant concentration in fat (mg/kg)}}{\text{daily contaminant intake (mg/d)}} \quad \text{(A-3)}$$

The biotransfer factors B_t and B_k for organic compounds can be estimated from the biotransfer factor B_f by multiplying B_f by the fat content of the milk or meat being considered. Whole milk has a fat content on the order of 4%. All dairy products including milks, cheeses, ice cream, cottage cheese, etc., have ingestion-weighted fat contents of from 4 to 6%. Meat derived from cattle has a fat content in the range 30 to 50%.

UPTAKE OF ORGANIC CHEMICALS IN FAT, MEAT, AND MILK

Kenaga (1980) reviewed bioconcentration factors in fat tissues derived from dietary feeding studies for 23 chemicals in cattle. Based on this review, Kenaga (1980) proposed a regression equation for estimating the

bioconcentration factor K_{fd} in terms of the dimensionless octanol/water partition coefficient K_{ow},

$$\log K_{fd} = (0.5 \log K_{ow} - 3.457) \pm 2.0 \quad n = 23,\ r = 0.79 \qquad \text{(A-4)}$$

The dimensionless fat/diet biotransfer factor, K_{fd} expresses the ratio of contaminant concentration in fat (mg/kg) to that in feed [mg/kg (dry mass)]. The factor ± 2 expresses the orders of magnitude containing the 95% confidence limits for predicted data about the mean of $\log K_{ow}$.

The bioconcentration factor K_{fd} can be converted to a biotransfer factor to fat by dividing K_{fd} by the animal's daily feed intake. Using 12 kg/d for beef cattle and 17 kg/d for dairy cattle (from Table 2-7), one obtains from Eq. A-4

$$\log B_f = (0.5 \log K_{ow} - 4.54) \pm 2 \qquad \text{(A-5)}$$
for beef cattle

$$\log B_f = (0.5 \log K_{ow} - 4.69) \pm 2 \qquad \text{(A-6)}$$
for dairy cattle

Multiplying B_f by the fat content of dairy products (~ 5%) and meat (~ 40%) converts Eqs. A-5 and A-6 into regression equations for the biotransfer factors B_t and B_k:

$$\log B_t = (0.5 \log K_{ow} - 4.94) \pm 2 \qquad \text{(A-7)}$$

$$\log B_k = (0.5 \log K_{ow} - 5.99) \pm 2 \qquad \text{(A-8)}$$

Travis and Arms (1988) have reviewed biotransfer factors for 36 chemicals in meat and 28 chemicals in milk. For each of these pathways they have developed geometric mean regressions for the biotransfer factors in terms of K_{ow}. Their proposed regression equations are

$$\log B_t = \log K_{ow} - 7.6 \quad n = 36,\ r = 0.81 \qquad \text{(A-9)}$$

$$\log B_k = \log K_{ow} - 8.1 \quad n = 28,\ r = 0.74 \qquad \text{(A-10)}$$

Travis and Arms (1988) have not estimated the uncertainty bounds on their estimates. The compounds studied by Travis and Arms had log K_{ow} in the range 1.3 to 6.9. Eqs. A-7 and A-9 give the same result when log K_{ow} = 5.3. Eqs. A-8 and A-10 give the same result when log K_{ow} = 4.2. When log K_{ow} = 1.3, the difference between log B_t estimated from Eqs. A-7 and A-9 is 2.0 (this is rather large and at the upper bound as expressed in Eq. A-7). Using log K_{ow} = 6.9 in Eqs. A-8 and A-10 gives a difference in the estimated value of B_k of 1.5.

Uptake of Chemical Elements in Meat and Milk

Ng (1982) has compiled values of B_t and B_k for several elements. His work indicates that there can be as much as an order of magnitude uncertainty in estimating these parameters. Table A-1 lists values of B_t and B_k compiled by Ng for elements likely to be found in hazardous wastes.

Table A-1. Elemental biotransfer factors for feed-to-milk and feed-to-beef as compiled by Ng (1982).

Element	B_k (d/L)	B_t (median) (d/kg)	B_t 95% interval
Antimony	1.1×10^{-4}	--	
Arsenic	6.2×10^{-5}	--	
Barium	3.5×10^{-4}	9.7×10^{-5}	1.7×10^{-5} to 5.6×10^{-4}
Beryllium	9.1×10^{-7}	--	
Calcium	1.1×10^{-2}	7.2×10^{-4}	2.0×10^{-4} to 2.5×10^{-3}
Cadmium	1.5×10^{-3}	--	
Cesium	7.1×10^{-3}	1.1×10^{-2}	4.7×10^{-3} to 9.7×10^{-2}
Chromium	1.1×10^{-3}	9.2×10^{-3}	7.6×10^{-4} to 1.1×10^{-1}
Copper	1.7×10^{-3}	1.3×10^{-2}	3.2×10^{-3} to 4.9×10^{-2}
Lead	2.6×10^{-4}	--	
Mercury	4.7×10^{-4}	--	
Nickel	1.0×10^{-3}	2.0×10^{-3}	3.4×10^{-4} to 1.1×10^{-2}
Radium	4.0×10^{-4}	5.0×10^{-4}	~ 0 to 2.0×10^{-3}
Selenium	4.0×10^{-3}	--	
Silver	1.3×10^{-2}	1.9×10^{-3}	3.3×10^{-4} to 1.1×10^{-2}
Strontium	1.4×10^{-3}	5.9×10^{-4}	6.3×10^{-5} to 5.5×10^{-3}
Thallium	1.9×10^{-3}	--	
Zinc	1.0×10^{-2}	1.2×10^{-1}	4.7×10^{-2} to 3.2×10^{-1}

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